PubChem

COMPOUND SUMMARY

Adiponitrile

PubChem CID	812
Structure	2D 3D Crystal
Chemical Safety	Acute Toxic Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_6H_8N_2$ $CN(CH_2)_4CN$
Synonyms	ADIPONITRILE Hexanedinitrile 1,4-Dicyanobutane 111-69-3 Adipyldinitrile View More...
Molecular Weight	108.14 g/mol *Computed by PubChem 2.2 (PubChem release 2021.10.14)*
Dates	Create: 2005-03-26 Modify: 2024-12-06
Description	Adiponitrile appears as a colorless to light yellow liquid which is fairly soluble and is less dense than water. Contact

may irritate skin, eyes and mucous membranes. May be toxic by ingestion, inhalation and skin absorption.

- CAMEO Chemicals

Adiponitrile is a chemical compound of cyanide. It is is an important precursor to the polymer nylon 66. (L584)

L584: Wikipedia. Adiponitrile. Last Updated 15 February 2009. ***http://en.wikipedia.org/wiki/Adiponitrile***

- Toxin and Toxin Target Database (T3DB)

See also: ... View More ...

Contents

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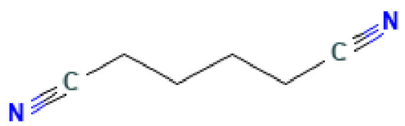
1 Structures

1.1 2D Structure

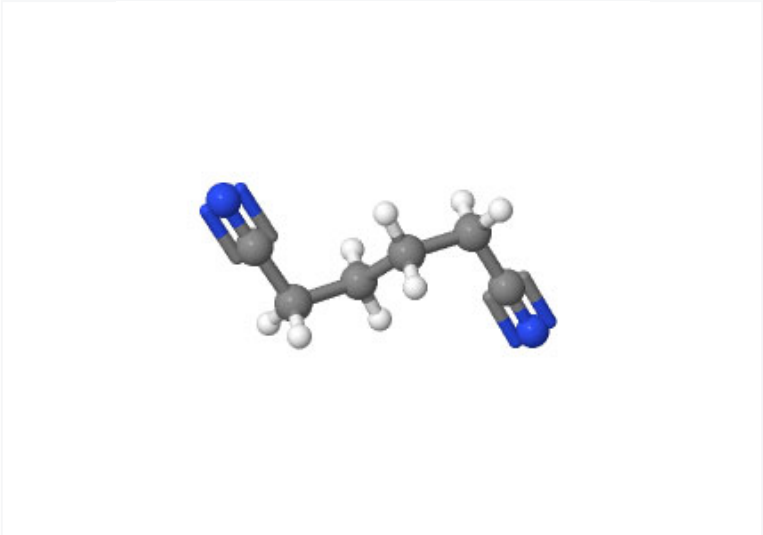
Chemical Structure Depiction



PubChem

1.2 3D Conformer

1.3 Crystal Structures

1 of 2	View All
COD Number	2020899
Associated Article	Seidel, Rüdiger W.; Goddard, Richard; Nöthling, Nils; Lehmann, Christian W.. Adiponitrile at 100K. Acta Crystallographica Section C 2017;73(11):937-940. DOI: 10.1107/S2053229617014620
Crystal Structure Depiction	
Hermann-Mauguin space group symbol	P 1 21/c 1
Hall space group symbol	-P 2ybc
Space group number	14
a	4.5031 Å
b	6.5860 Å
c	10.572 Å
α	90 °

β	96.540 °
γ	90 °
Z	2
Z'	0.5
Residual factor	0.0456

Crystallography Open Database (COD)

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

hexanedinitrile

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

PubChem

2.1.2 InChI

InChI=1S/C6H8N2/c7-5-3-1-2-4-6-8/h1-4H2

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

PubChem

2.1.3 InChIKey

BTGRAWJCKBQKAO-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

PubChem

2.1.4 SMILES

C(CCC#N)CC#N

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

- PubChem

2.2 Molecular Formula

$C_6H_8N_2$

Computed by PubChem 2.2 (PubChem release 2021.10.14)

- Australian Industrial Chemicals Introduction Scheme (AICIS); CAMEO Chemicals; PubChem

$C_6H_8N_2$

$CN(CH_2)_4CN$

- ILO-WHO International Chemical Safety Cards (ICSCs)

2.3 Other Identifiers

2.3.1 CAS

111-69-3

- Australian Industrial Chemicals Introduction Scheme (AICIS); CAMEO Chemicals; CAS Common C...

68411-90-5

- ChemIDplus

2.3.2 Deprecated CAS

55462-97-0

- ChemIDplus; EPA Chemicals under the TSCA

68511-79-5

- ChemIDplus

2.3.3 European Community (EC) Number

203-896-3

- European Chemicals Agency (ECHA)

2.3.4 UNII

SYT33B891I

- FDA Global Substance Registration System (GSRS)

2.3.5 UN Number

2205 (ADIPONITRILE)

- CAMEO Chemicals; Emergency Response Guidebook (ERG)

2205

- ILO-WHO International Chemical Safety Cards (ICSCs); The National Institute for Occupational Sa...

2.3.6 ChEMBL ID

CHEMBL2132938

- ChEMBL

2.3.7 DSSTox Substance ID

DTXSID3021936

- EPA DSSTox

2.3.8 HMDB ID

HMDB0248015

- Human Metabolome Database (HMDB)

2.3.9 ICSC Number

0211

- ILO-WHO International Chemical Safety Cards (ICSCs)

2.3.10 Nikkaji Number

J2.456B

- Japan Chemical Substance Dictionary (Nikkaji)

2.3.11 NSC Number

7617

- DTP/NCI

2.3.12 RTECS Number

AV2625000

- The National Institute for Occupational Safety and Health (NIOSH)

2.3.13 Wikidata

Q84062

- Wikidata

2.3.14 Wikipedia

Adiponitrile

- Wikipedia

2.4 Synonyms

2.4.1 MeSH Entry Terms

adiponitrile

hexanedinitrile

Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

ADIPONITRILE	Adipic acid nitrile	Adipinsaeuredinitril [German]	AI3-11080
Hexanedinitrile	Hexanedioic acid, dinitrile	CAS-111-69-3	EINECS 270-153
1,4-Dicyanobutane	NSC 7617	CCRIS 4570	Adiponitrile, 99
111-69-3	MFCD00001975	HSDB 627	hexane-1,6-dini
Adipyldinitrile	SYT33B891I	EINECS 203-896-3	ADIPONITRILE
Adipodinitrile	DTXSID3021936	Hexanedioic acid dinitrile	BUTANEDICARI
Adipic acid dinitrile	NSC-7617	UN2205	WLN: NC4CN
Tetramethylene dicyanide	Adipinsaeuredinitril	BRN 1740005	ADIPONITRILE
Nitrile adipico	DTXCID201936	UNII-SYT33B891I	EC 203-896-3
Tetramethylene cyanide	Nitrile adipico [Italian]	Adipic dinitrile	SCHEMBL5934(

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	108.14 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
XLogP3	-0.3	Computed by XLogP3 3.0 (PubChem release 2021.10.14)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Hydrogen Bond Acceptor Count	2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Rotatable Bond Count	3	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Exact Mass	108.068748264 Da	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Monoisotopic Mass	108.068748264 Da	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Topological Polar Surface Area	47.6Å^2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Heavy Atom Count	8	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	113	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.10.14)

PubChem

3.2 Experimental Properties

3.2.1 Physical Description

Adiponitrile appears as a colorless to light yellow liquid which is fairly soluble and is less dense than water. Contact may irritate skin, eyes and mucous membranes. May be toxic by ingestion, inhalation and skin absorption.

CAMEO Chemicals

Liquid

- EPA Chemical Data Reporting (CDR)

Water-white, practically odorless, oily liquid;[Note: A solid below 34 degrees F; Forms cyanide in the body; [NIOSH]

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

ODOURLESS OILY COLOURLESS LIQUID.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Water-white, practically odorless, oily liquid.

- Occupational Safety and Health Administration (OSHA)

Water-white, practically odorless, oily liquid. [Note: A solid below 34 °F. Forms cyanide in the body.]

- The National Institute for Occupational Safety and Health (NIOSH)

3.2.2 Color / Form

NEEDLES FROM ETHER

Lide, D.R. (ed). CRC Handbook of Chemistry and Physics. 72nd ed. Boca Raton, FL: CRC Press, 1991-1992., p. 3-29

- Hazardous Substances Data Bank (HSDB)

Colorless liq

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3152

- Hazardous Substances Data Bank (HSDB)

Water-white, oily liquid

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 8

- Hazardous Substances Data Bank (HSDB)

3.2.3 Odor

Practically odorless.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 8

- **Hazardous Substances Data Bank (HSDB)**

3.2.4 Boiling Point

563 °F at 760 mmHg (EPA, 1998)

U.S. Environmental Protection Agency. 1998. Extremely Hazardous Substances (EHS) Chemical Profiles and Emergency First Aid Guides. Washington, D.C.: U.S. Government Printing Office.

- **CAMEO Chemicals**

295 °C @ 760 mm Hg

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 23

- **Hazardous Substances Data Bank (HSDB)**

295 °C

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

563 °F

- **Occupational Safety and Health Administration (OSHA); The National Institute for Occupational S…**

3.2.5 Melting Point

36.1 °F (EPA, 1998)

U.S. Environmental Protection Agency. 1998. Extremely Hazardous Substances (EHS) Chemical Profiles and Emergency First Aid Guides. Washington, D.C.: U.S. Government Printing Office.

- **CAMEO Chemicals**

1-3 °C

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 23

- **Hazardous Substances Data Bank (HSDB)**

1 °C

- ILO-WHO International Chemical Safety Cards (ICSCs)

34 °F

- Occupational Safety and Health Administration (OSHA); The National Institute for Occupational S...

3.2.6 Flash Point

199.4 °F (EPA, 1998)

U.S. Environmental Protection Agency. 1998. Extremely Hazardous Substances (EHS) Chemical Profiles and Emergency First Aid Guides. Washington, D.C.: U.S. Government Printing Office.

- CAMEO Chemicals

93 °C

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

200 °F (93 °C) (OPEN CUP)

Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 325-11

- Hazardous Substances Data Bank (HSDB)

159 °C c.c.

- ILO-WHO International Chemical Safety Cards (ICSCs)

199 °F (open cup)

- Occupational Safety and Health Administration (OSHA)

(oc) 199 °F

- The National Institute for Occupational Safety and Health (NIOSH)

3.2.7 Solubility

50 to 100 mg/mL at 73 °F (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North

Carolina.

▸ CAMEO Chemicals

Sol in alc, chloroform

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 23

▸ Hazardous Substances Data Bank (HSDB)

Sol in methanol, ethanol, chloroalkanes, and aromatics but has low solubility in carbon disulfide, ethyl ether, and aliphatic hydrocarbons.

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. SUPP (1998) 444

▸ Hazardous Substances Data Bank (HSDB)

In water, 8.0X10+4 mg/l @ 20 °C.

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. SUPP (1998) 444

▸ Hazardous Substances Data Bank (HSDB)

Solubility in water, g/l at 20 °C: 50-100 (good)

▸ ILO-WHO International Chemical Safety Cards (ICSCs)

4.5%

▸ The National Institute for Occupational Safety and Health (NIOSH)

3.2.8 Density

0.965 at 68 °F (EPA, 1998) - Less dense than water; will float

U.S. Environmental Protection Agency. 1998. Extremely Hazardous Substances (EHS) Chemical Profiles and Emergency First Aid Guides. Washington, D.C.: U.S. Government Printing Office.

▸ CAMEO Chemicals

0.9676 g/ml @ 20 °C

Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 81st Edition. CRC Press LLC, Boca Raton: FL 2000, p. 3-187

▸ Hazardous Substances Data Bank (HSDB)

Relative density (water = 1): 0.97

- ILO-WHO International Chemical Safety Cards (ICSCs)

0.97

- Occupational Safety and Health Administration (OSHA); The National Institute for Occupational S...

3.2.9 Vapor Density

3.73 (EPA, 1998) - Heavier than air; will sink (Relative to Air)

U.S. Environmental Protection Agency. 1998. Extremely Hazardous Substances (EHS) Chemical Profiles and Emergency First Aid Guides. Washington, D.C.: U.S. Government Printing Office.

- CAMEO Chemicals

3.73 (air= 1)

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3152

- Hazardous Substances Data Bank (HSDB)

Relative vapor density (air = 1): 3.7

- ILO-WHO International Chemical Safety Cards (ICSCs)

3.73

- Occupational Safety and Health Administration (OSHA)

3.2.10 Vapor Pressure

2 mmHg at 246 °F (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

- CAMEO Chemicals

0.000679 [mmHg]

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

6.8X10-4 mm Hg at 25 °C

Daubert, T.E., R.P. Danner. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, D.C.: Taylor and Francis, 1989.

- **Hazardous Substances Data Bank (HSDB)**

Vapor pressure, Pa at 20 °C: 0.3

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

0.002 mmHg

- **Occupational Safety and Health Administration (OSHA); The National Institute for Occupational S...**

3.2.11 LogP

log Kow= -0.32

PMID:4026577

Tanii H, Hashimoto K; Arch Toxicol 57: 88-93 (1985)

- **Hazardous Substances Data Bank (HSDB)**

-0.32

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

3.2.12 Autoignition Temperature

1022 °F (USCG, 1999)

U.S. Coast Guard. 1999. Chemical Hazard Response Information System (CHRIS) - Hazardous Chemical Data. Commandant Instruction 16465.12C. Washington, D.C.: U.S. Government Printing Office.

- **CAMEO Chemicals**

1022 °F (550 °C)

Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 49-13

- **Hazardous Substances Data Bank (HSDB)**

550 °C

- ILO-WHO International Chemical Safety Cards (ICSCs)

3.2.13 Decomposition

WHEN HEATED TO DECOMP RELEASES VAPORS CONTAINING HYDROCYANIC ACID.

Winek, C.L. Drug and Chemical Blood-Level Data 1985. Pittsburgh, PA: Allied Fischer Scientific, 1985., p. 938

- Hazardous Substances Data Bank (HSDB)

When heated to decomp it emits highly toxic fumes of CN- /cyanides/.

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 73

- Hazardous Substances Data Bank (HSDB)

3.2.14 Viscosity

9.1 cP @ 20 °C; 2.6 cP @ 70 °C

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. SUPP (1998) 445

- Hazardous Substances Data Bank (HSDB)

58 mPa*s at 30 °C

- ILO-WHO International Chemical Safety Cards (ICSCs)

3.2.15 Heat of Combustion

-40.4X10+6 J/kg

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. SUPP (1998) 445

- Hazardous Substances Data Bank (HSDB)

3.2.16 Heat of Vaporization

70.4X10+4 J/kg

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. SUPP (1998) 445

- Hazardous Substances Data Bank (HSDB)

3.2.17 Refractive Index

Index of refraction: 1.4380 @ 20 °C/D

Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 81st Edition. CRC Press LLC, Boca Raton: FL 2000, p. 3-187

- Hazardous Substances Data Bank (HSDB)

3.2.18 Kovats Retention Index

Standard non-polar	1090

- NIST Mass Spectrometry Data Center

3.2.19 Other Experimental Properties

Vap: 2 mm Hg @ 119 °C

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3152

- Hazardous Substances Data Bank (HSDB)

3.3 SpringerMaterials Properties

Boiling point
Density
Dielectric constant
Excess enthalpy
Heat of solution
Heat of sublimation
Mixing enthalpy
Nuclear quadrupole resonance spectroscopy
Optical coefficient
Quadrupole coupling
Refractive index
Surface tension
Vapor pressure
Viscosity

- SpringerMaterials

3.4 Chemical Classes

Nitrogen Compounds -> Nitriles

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

4 Spectral Information

4.1 1D NMR Spectra

1 of 2	
1D NMR Spectra	1H NMR: SAD 6702 (Sadtler Research Laboratories spectral collection)

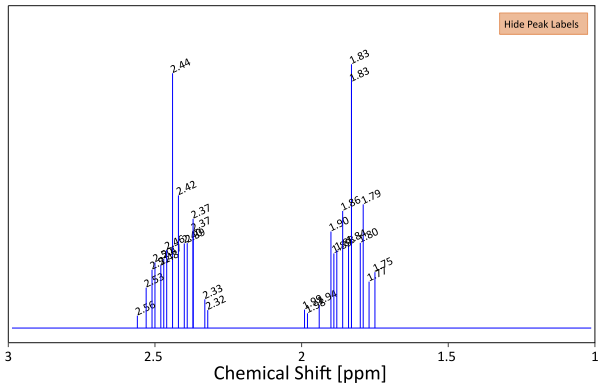
- Hazardous Substances Data Bank (HSDB)

2 of 2	
1D NMR Spectra	NMRShiftDB Link

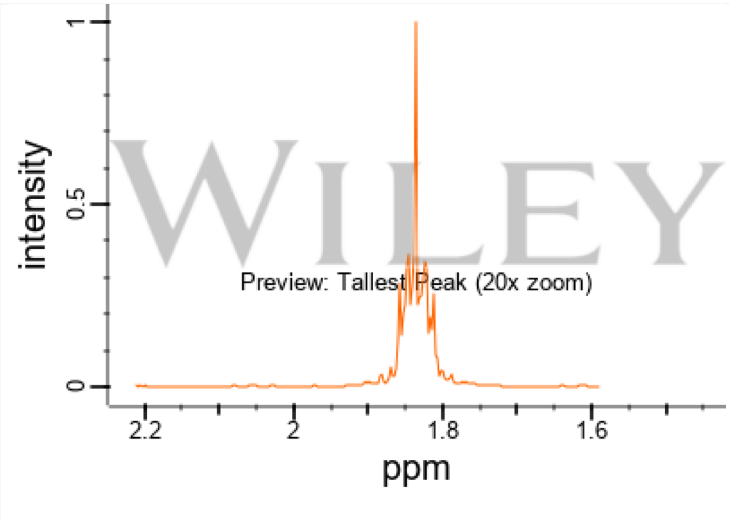
- NMRShiftDB

4.1.1 1H NMR Spectra

1 of 3	View All
Spectra ID	2155
Instrument Type	JEOL
Frequency	90 MHz
Solvent	CDCl3
Shifts [ppm]:Intensity	2.50:249.00, 1.99:70.00, 1.90:366.00, 2.33:109.00, 1.77:176.00, 2.47:263.00, 2.37:366.00, 1.80:323.00, 2.44:966.00, 2.56:47.00, 1.79:469.00, 1.94:88.00, 1.84:318.00, 1.89:283.00, 1.83:1000.00, 2.39:322.00, 1.88:294.00, 2.40:321.00, 2.51:221.00, 2.46:296.00,

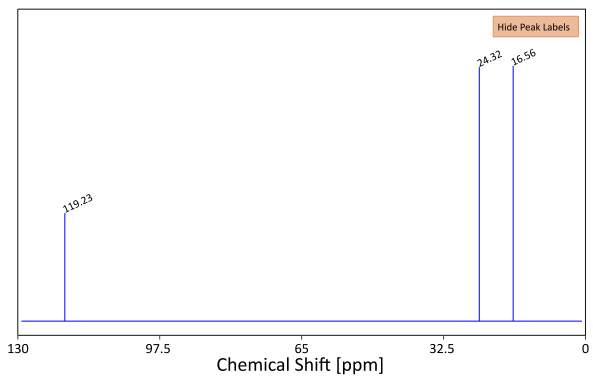
	2.53:153.00, 1.83:933.00, 2.37:414.00, 2.48:238.00, 2.32:68.00, 2.42:503.00, 1.75:212.00, 1.86:444.00, 1.98:56.00
Thumbnail	

▸ Human Metabolome Database (HMDB)

2 of 3	View All
Instrument Name	BRUKER AC-300
Source of Sample	Tokyo Kasei Kogyo Company, Ltd., Tokyo, Japan
Copyright	Copyright © 1991-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

▸ SpectraBase

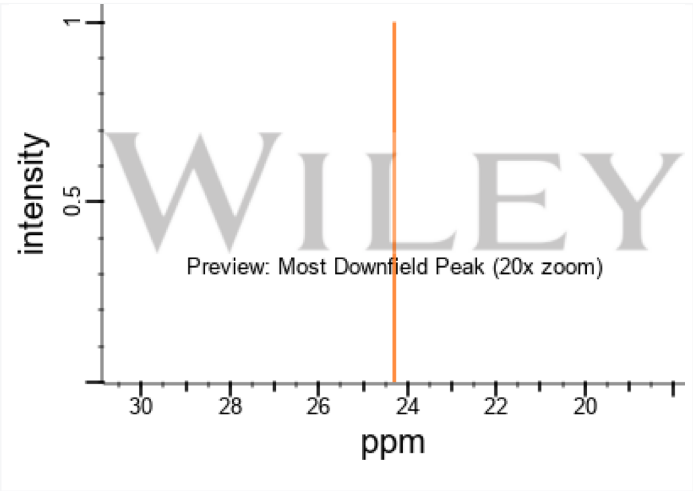
4.1.2 13C NMR Spectra

1 of 3	View All
Spectra ID	2842
Instrument Type	Varian
Frequency	25.16 MHz
Solvent	CDCl3
Shifts [ppm]:Intensity	119.23:423.00, 24.32:995.00, 16.56:1000.00
Thumbnail	

Human Metabolome Database (HMDB)

2 of 3	View All
Source of Sample	Tokyo Kasei Kogyo Company, Ltd., Tokyo, Japan
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail



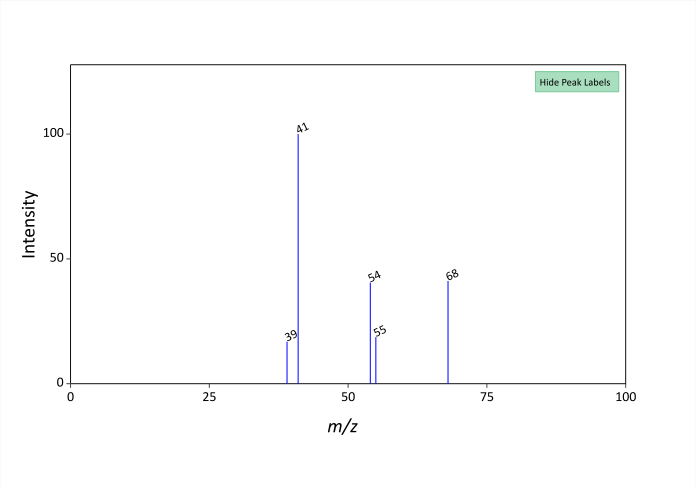
SpectraBase

4.2 Mass Spectrometry

4.2.1 GC-MS

1 of 7 View All

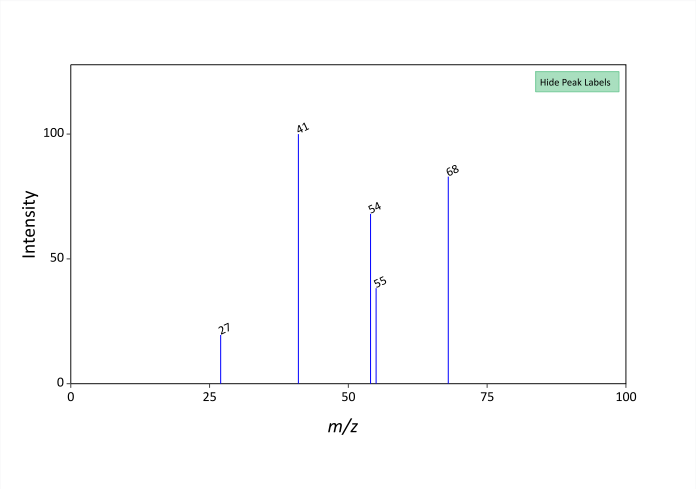
MoNA ID	JP004298
MS Category	Experimental
MS Type	GC-MS
MS Level	MS1
Instrument	HITACHI RMU-7M
Instrument Type	EI-B
Ionization Mode	positive
Top 5 Peaks	41 99.99 68 41.16 54 40.53 55 18.66 39 16.85
SPLASH	splash10-0006-9000000000-811971dea62fd0719211

Thumbnail	
License	CC BY-NC-SA

MassBank of North America (MoNA)

2 of 7 View All

MoNA ID	JP007368
MS Category	Experimental
MS Type	GC-MS
MS Level	MS1
Instrument	HITACHI RMU-6M
Instrument Type	EI-B
Ionization Mode	positive
Top 5 Peaks	41 99.99 68 82.95 54 68.04 55 38.27 27 19.52
SPLASH	splash10-0fr6-9000000000-fa4c798c5039209f7367

Thumbnail	
License	CC BY-NC-SA

▸ MassBank of North America (MoNA)

4.2.2 Other MS

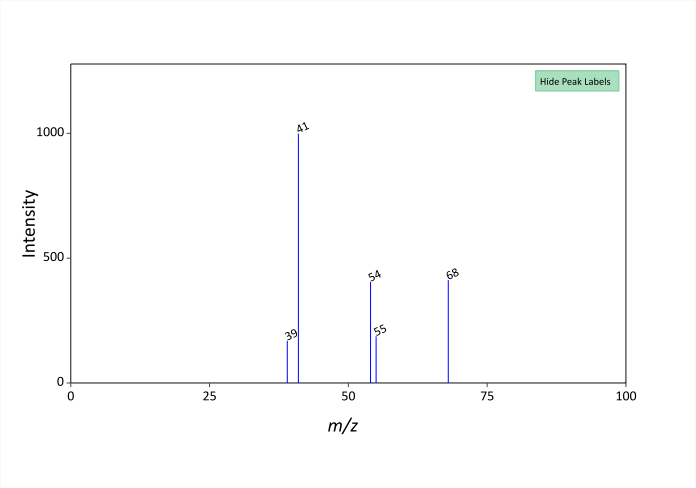
1 of 3 View All

Other MS	MS: NIST 1422 (NIST/EPA/MSDC Mass Spectral database, 1990 version); WILEY 510 (Atlas of Mass Spectral Data, John Wiley and Sons, New York)

▸ Hazardous Substances Data Bank (HSDB)

2 of 3 View All

Accession ID	MSBNK-Fac_Eng_Univ_Tokyo-JP004298
Authors	TAJIMA S, GUNMA COLLEGE OF TECHNOLOGY
Instrument	HITACHI RMU-7M
Instrument Type	EI-B
MS Level	MS
Ionization Mode	POSITIVE
Ionization	ENERGY 70 eV

Top 5 Peaks	41 999 68 412 54 405 55 187 39 169
SPLASH	splash10-0006-9000000000-811971dea62fd0719211
Thumbnail	
License	CC BY-NC-SA

▸ MassBank Europe

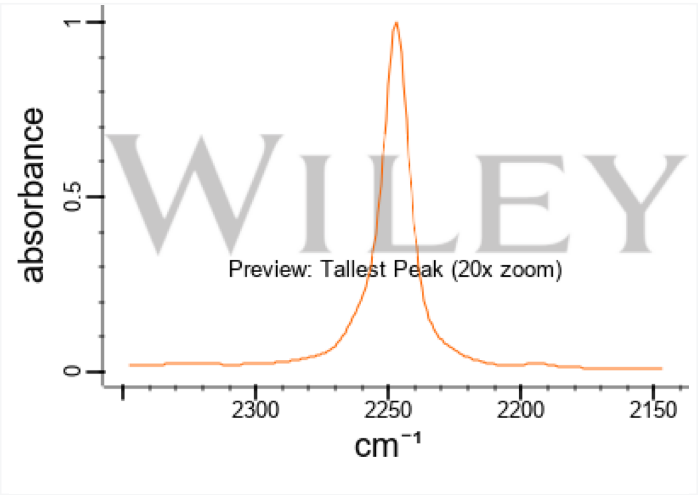
4.3 IR Spectra

IR Spectra	IR: SADG 1875 (Sadtler Research Laboratories IR grating Collection)

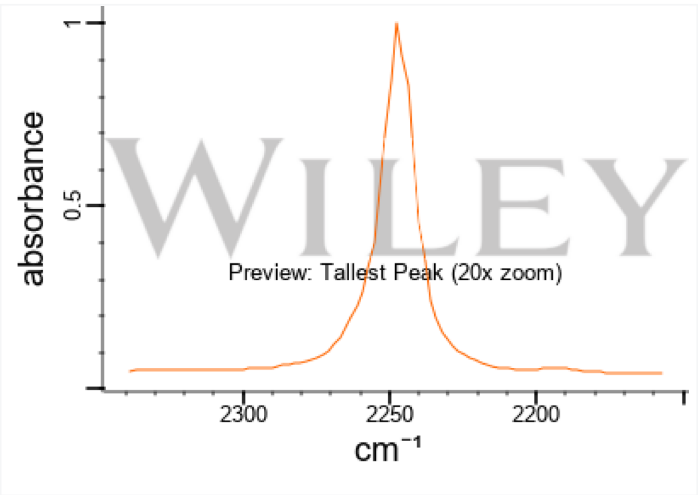
▸ Hazardous Substances Data Bank (HSDB)

4.3.1 FTIR Spectra

1 of 2	
Technique	NEAT
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.

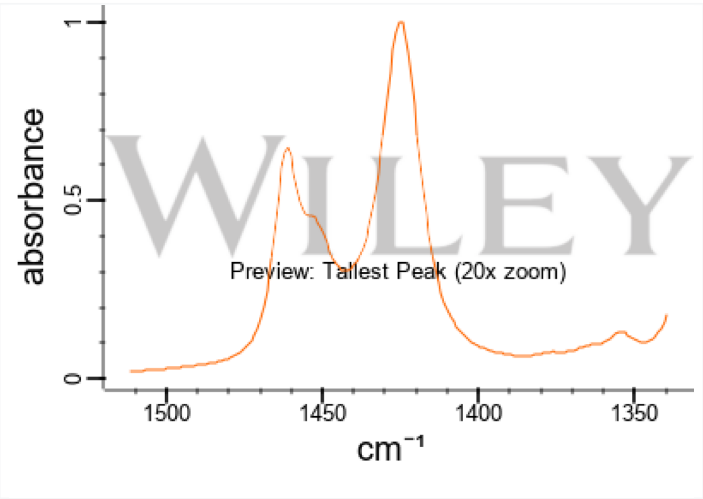
Thumbnail	

▸ SpectraBase

2 of 2	
Instrument Name	Bruker IFS 85
Technique	Cell
Copyright	Copyright © 1989, 1990-2024 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
Thumbnail	

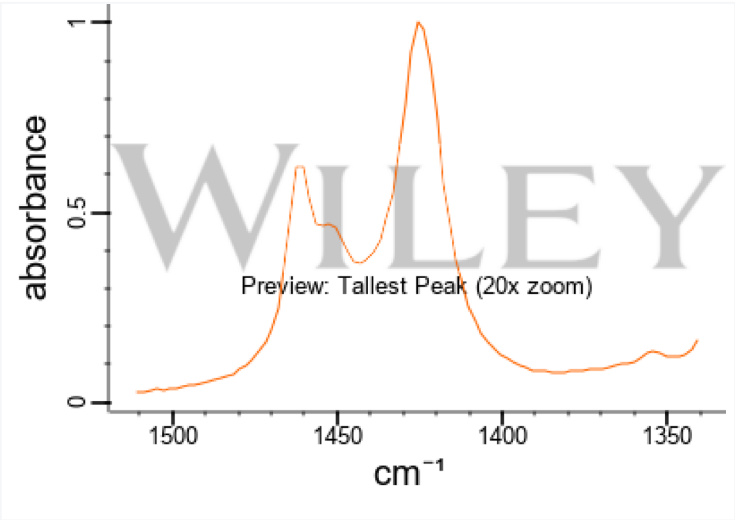
▸ SpectraBase

4.3.2 ATR-IR Spectra

1 of 2	
Technique	ATR-Cylindrical Internal Reflectance (CIR)
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

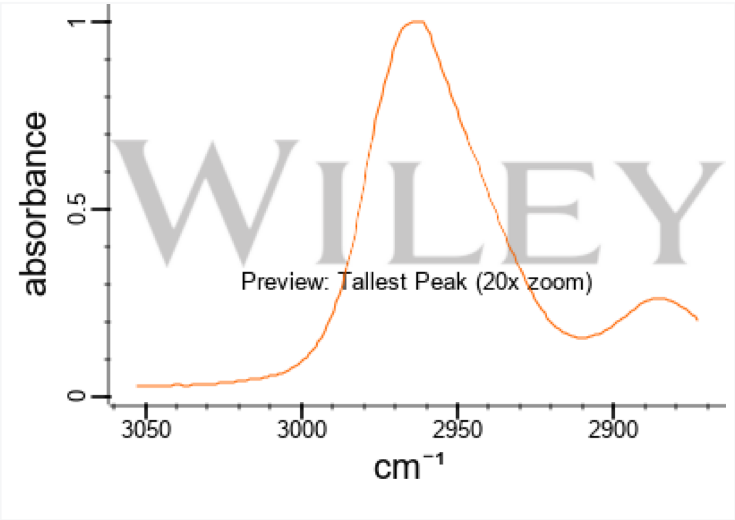
SpectraBase

2 of 2	
Source of Sample	Aldrich
Catalog Number	D77001
Copyright	Copyright © 2018-2024 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2018-2024 John Wiley & Sons, Inc. All Rights Reserved.

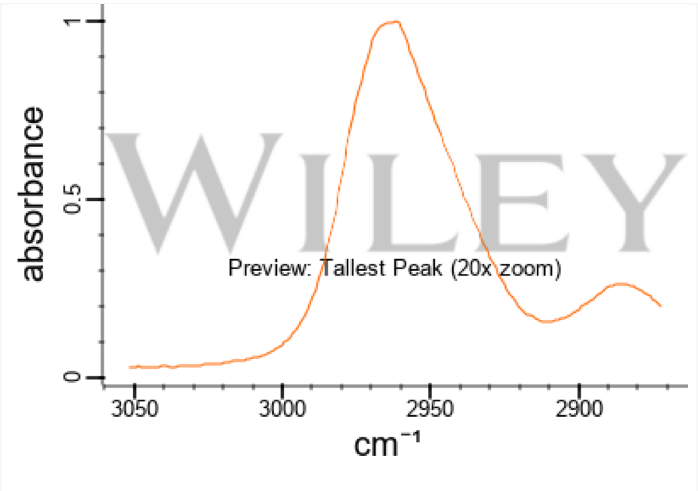
Thumbnail	

SpectraBase

4.3.3 Vapor Phase IR Spectra

1 of 2	
Technique	Vapor Phase
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

2 of 2	
Instrument Name	DIGILAB FTS-14
Technique	Vapor Phase
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

- SpectraBase

5 Related Records

5.1 Related Compounds with Annotation

Follow these links to do a live 2D search or do a live 3D search for this compound, sorted by annotation score. This section is deprecated (see here for details), but these live search links provide equivalent functionality to the table that was previously shown here.

- PubChem

5.2 Related Compounds

Same Connectivity Count	2
Same Parent, Connectivity Count	17

Same Parent, Exact Count	16
Mixtures, Components, and Neutralized Forms Count	94
Similar Compounds (2D)	View in PubChem Search
Similar Conformers (3D)	View in PubChem Search

PubChem

5.3 Substances

5.3.1 Related Substances

All Count	283
Same Count	146
Mixture Count	137

PubChem

5.3.2 Substances by Category

PubChem

5.4 Other Relationships

Hexanedinitrile, hydrogenated, high-boiling fraction (annotation moved to)

- PubChem

5.5 Entrez Crosslinks

PubMed Count	20

- PubChem

6 Chemical Vendors

- PubChem

7 Drug and Medication Information

7.1 Reported Fatal Dose

205 to 300 milligrams for an adult human (cyanide salts). (T86)

T86: Baselt RC and Cravey RH (1989). Disposition of Toxic Drugs and Chemicals in Man. 3rd ed. Chicago, IL.: Year Book Medical Publishers.

- Toxin and Toxin Target Database (T3DB)

8 Pharmacology and Biochemistry

8.1 Absorption, Distribution and Excretion

Seventy nine percent of dose /about 50 mg/kg sc admin to guinea pigs/ was eliminated as **thiocyanate** in urine. ... Skin penetration was suggested by incr in **thiocyanate** in urine ... after application to depilated skin. Greater quantities were absorbed when skin was abraded.

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3152

- Hazardous Substances Data Bank (HSDB)

The concentrations of **thiocyanate** in the blood and urine of guinea pigs injected with adiponitrile were proportional to the doses administered. Following administration of adiponitrile, 79% was eliminated as **thiocyanate** in the urine of guinea pigs. Of the **cyanide** antidotes, **thiosulfate** was most effective. However, on the basis of the ratio between administered adiponitrile dose and quantity of **cyanide** detected, /it was/ concluded that a greater part of the dose was metabolized to **cyanide**.

Snyder, R. (ed.). Ethel Browning's Toxicity and Metabolism of Industrial Solvents. 2nd ed. Volume II: Nitrogen and Phosphorus Solvents. Amsterdam-New York-Oxford: Elsevier, 1990., p. 325

- Hazardous Substances Data Bank (HSDB)

8.2 Metabolism / Metabolites

... In guinea pigs ... it is hydrolyzed to **hydrogen cyanide** in the body giving rise to **thiocyanate** in urine.

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3152

- Hazardous Substances Data Bank (HSDB)

Male ddY mice were pretreated with **carbon tetrachloride** or olive oil and administered adiponitrile orally in concentrations sufficient to determine its median lethal dose (LD50). Brain **cyanide** concentrations were determined. The distribution coefficient (P) for partitioning adiponitrile between **water** and **n-octanol** was measured. Mice were pretreated as before and dosed with adiponitrile at 3 to 5 times its LD50. Mean survival times were determined. Hepatic microsomes were obtained from mice pretreated with **carbon tetrachloride** or olive oil and

incubated with adiponitrile. The rate of release of free **cyanide** was investigated. The oral LD50 for animals pretreated with olive oil was 1.592 mmol/kg. The LD50 for the **carbon tetrachloride** treated mice was 2.652 mmol/kg. Brain **cyanide** concentrations in olive oil pretreated mice ranged from 0.35 to 0.74 ug/g. **Carbon tetrachloride** pretreatment lengthened survival and reduced brain **cyanide** concentrations. Dinitriles are metabolized to cyanides in vivo and in vitro.

Tanii H, Hashimoto K; Archives of Toxicol 57 (2): 88-93 (1985)

- **Hazardous Substances Data Bank (HSDB)**

Organic nitriles are converted into **cyanide** ions through the action of cytochrome P450 enzymes in the liver. **Cyanide** is rapidly absorbed and distributed throughout the body. **Cyanide** is mainly metabolized into **thiocyanate** by either rhodanese or **3-mercaptopyruvate sulfur** transferase. **Cyanide** metabolites are excreted in the urine. (L96)

L96: ATSDR - Agency for Toxic Substances and Disease Registry (2006). Toxicological profile for cyanide. U.S. Public Health Service in collaboration with U.S. Environmental Protection Agency (EPA). ***http://www.atsdr.cdc.gov/toxprofiles/tp8.html***

- **Toxin and Toxin Target Database (T3DB)**

9 Use and Manufacturing

9.1 Uses

Sources/Uses

Used to manufacture **hexamethylenediamine** that is used to make nylon 66; [HSDB]

- **Haz-Map, Information on Hazardous Chemicals and Occupational Diseases**

Intermediate in the manufacture of nylon; organic synthesis

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 23

- **Hazardous Substances Data Bank (HSDB)**

Preparation of adipoquanamine; extractant for aromatic hydrocarbons

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. SUPP (1998) 447

- **Hazardous Substances Data Bank (HSDB)**

9.1.1 Use Classification

Hazard Classes and Categories -> Flammable - 2nd degree, Reactive - 1st degree

- NJDOH RTK Hazardous Substance List

9.1.2 Industry Uses

Other (specify)
Intermediates
Intermediate

https://www.epa.gov/chemical-data-reporting

- EPA Chemical Data Reporting (CDR)

9.2 Methods of Manufacturing

Chlorination of butadiene to dichlorobutylene, which is reacted with 35% sodium cyanide soln to yield 1,4-dicyanobutylene; which is hydrogenated to adiponitrile. Also by electroorganic synthesis from acrylonitrile.

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 23

- Hazardous Substances Data Bank (HSDB)

Reaction of adipic acid with ammonia (either liquid or vapor phase) produces adipamide as intermediate, which is subsequently dehydrated to adiponitrile.

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. SUPP (1998) 444

- Hazardous Substances Data Bank (HSDB)

Prepared by dimerization of acrylonitrile at the cathode of an electrolytic cell (propionitrile and bis(cyanoethyl) ether are by-products).

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. SUPP (1998) 446

- Hazardous Substances Data Bank (HSDB)

Prepared by direct addition of **hydrogen cyanide** to **butadiene** catalyzed by soluble, air and moisture sensitive, triarylphosphite nickel(0) complexes.

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. SUPP (1998) 446

- **Hazardous Substances Data Bank (HSDB)**

9.3 Impurities

Impurities that may be present /such as **propionitrile** and bis(cyanoethyl) ether in the **butadiene** process and **acrylonitrile** in the electrolytic process/ depend on the method of manufacture and, thus, vary depending on the source.

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. SUPP (1998) 446

- **Hazardous Substances Data Bank (HSDB)**

9.4 Formulations / Preparations

Typical concentration is 99.5 wt% adiponitrile

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. SUPP (1998) 446

- **Hazardous Substances Data Bank (HSDB)**

9.5 U.S. Production

Aggregated Product Volume

2019: 1,000,000,000 - <5,000,000,000 lb

2018: 1,000,000,000 - <5,000,000,000 lb

2017: 1,000,000,000 - <5,000,000,000 lb

2016: 1,000,000,000 - <5,000,000,000 lb

https://www.epa.gov/chemical-data-reporting

- **EPA Chemical Data Reporting (CDR)**

(1972) 3.6X10+11 GRAMS

SRI

- Hazardous Substances Data Bank (HSDB)

(1991) 1415 million lb (capacity)

SRI. 1992 Directory of Chemical Producers-United States of America. Menlo Park, CA: SRI International, 1992., p. 444

- Hazardous Substances Data Bank (HSDB)

U.S. production capacity = 625,000 metric tons in 1992

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. SUPP (1998) 447

- Hazardous Substances Data Bank (HSDB)

9.6 General Manufacturing Information

Industry Processing Sectors

All Other Basic Organic Chemical Manufacturing
All Other Chemical Product and Preparation Manufacturing
Services

- EPA Chemical Data Reporting (CDR)

EPA TSCA Commercial Activity Status

Hexanedinitrile: ACTIVE

- EPA Chemicals under the TSCA

10 Identification

10.1 Analytic Laboratory Methods

A GC method ... using a flame ionization detector and SP1000 column.

Snyder, R. (ed.). Ethel Browning's Toxicity and Metabolism of Industrial Solvents. 2nd ed. Volume II: Nitrogen and Phosphorus Solvents. Amsterdam-New York-Oxford: Elsevier, 1990., p. 325

- Hazardous Substances Data Bank (HSDB)

11 Safety and Hazards

11.1 Hazards Identification

1.1.1 GHS Classification

1 of 3 View All

Pictogram(s)	Acute Toxic Irritant
Signal	Danger
GHS Hazard Statements	H301 (100%): Toxic if swallowed [**Danger** Acute toxicity, oral] H315 (19.9%): Causes skin irritation [**Warning** Skin corrosion/irritation] H319 (20.4%): Causes serious eye irritation [**Warning** Serious eye damage/eye irritation] H330 (20.4%): Fatal if inhaled [**Danger** Acute toxicity, inhalation] H332 (77.7%): Harmful if inhaled [**Warning** Acute toxicity, inhalation] H335 (19.9%): May cause respiratory irritation [**Warning** Specific target organ toxicity, single exposure; Respiratory tract irritation]
Precautionary Statement Codes	P260, P261, P264, P264+P265, P270, P271, P280, P284, P301+P316, P302+P352, P304+P340, P305+P351+P338, P316, P317, P319, P320, P321, P330, P332+P317, P337+P317, P362+P364, P403+P233, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided per 206 reports by companies from 7 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

European Chemicals Agency (ECHA)

11.1.2 Hazard Classes and Categories

Acute Tox. 3 (100%)

Skin Irrit. 2 (19.9%)

Eye Irrit. 2 (20.4%)

Acute Tox. 2 (20.4%)

Acute Tox. 4 (77.7%)

STOT SE 3 (19.9%)

- European Chemicals Agency (ECHA)

Acute toxicity (Oral) - Category 3

Acute toxicity (Dermal) - Category 3

Acute toxicity (Inhalation: Dusts and mists) - Category 4

Serious eye damage/eye irritation - Category 2B

Specific target organ toxicity - Single exposure - Category 1 (nervous system)

Specific target organ toxicity - Repeated exposure - Category 2 (blood)

- NITE-CMC

View More...

11.1.3 NFPA Hazard Classification

1 of 2 View All

NFPA 704 Diamond	2-2-1
NFPA Health Rating	2 - Materials that, under emergency conditions, can cause temporary incapacitation or residual injury.
NFPA Fire Rating	2 - Materials that must be moderately heated or exposed to relatively high ambient temperatures before ignition can occur. Materials would not under normal conditions form hazardous atmospheres with air, but under high ambient temperatures or under moderate heating could release vapor in sufficient quantities to produce hazardous atmospheres with air.

NFPA Instability Rating	1 - Materials that in themselves are normally stable but that can become unstable at elevated temperatures and pressures.

▸ Hazardous Substances Data Bank (HSDB)

11.1.4 Health Hazards

This material is toxic by ingestion and inhalation. It produces disturbances of the respiration and circulation, irritation of the stomach and intestine, and loss of weight. It is irritating to skin and eyes. (EPA, 1998)

U.S. Environmental Protection Agency. 1998. Extremely Hazardous Substances (EHS) Chemical Profiles and Emergency First Aid Guides. Washington, D.C.: U.S. Government Printing Office.

▸ CAMEO Chemicals

ERG 2024, Guide 153 (Adiponitrile)

· TOXIC and/or CORROSIVE; inhalation, ingestion or skin contact with material may cause severe injury or death.

· Methyl bromoacetate (UN2643) is an eye irritant/lachrymator (causes flow of tears).

· Contact with molten substance may cause severe burns to skin and eyes.

· Avoid any skin contact.

· Fire may produce irritating, corrosive and/or toxic gases.

· Runoff from fire control or dilution water may be corrosive and/or toxic and cause environmental contamination.

▸ Emergency Response Guidebook (ERG)

11.1.5 Fire Hazards

Combustion products may contain hydrogen cyanide (hydrocyanic acid, HCN). Vapor may explode if ignited in an enclosed area. When heated to decomposition, it emits highly toxic fumes. Avoid oxidizing material. Hazardous polymerization may not occur. (EPA, 1998)

U.S. Environmental Protection Agency. 1998. Extremely Hazardous Substances (EHS) Chemical Profiles and Emergency First Aid Guides. Washington, D.C.: U.S. Government Printing Office.

▸ CAMEO Chemicals

ERG 2024, Guide 153 (Adiponitrile)

· Combustible material: may burn but does not ignite readily.

· When heated, vapors may form explosive mixtures with air: indoors, outdoors and sewers explosion hazards.

· Those substances designated with a (P) may polymerize explosively when heated or involved in a fire.

· Corrosives in contact with metals may evolve flammable **hydrogen** gas.

· Containers may explode when heated.

· Runoff may pollute waterways.

· Substance may be transported in a molten form.

- **Emergency Response Guidebook (ERG)**

Combustible. Gives off irritating or toxic fumes (or gases) in a fire.

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

11.1.6 Hazards Summary

Toxic by ingestion; Skin burns in workers reported; [ACGIH] See NITRILES.

ACGIH - Documentation of the TLVs and BEIs, 7th Ed. Cincinnati: ACGIH Worldwide, 2020.

- **Haz-Map, Information on Hazardous Chemicals and Occupational Diseases**

11.1.7 Fire Potential

FLAMMABLE WHEN EXPOSED TO HEAT OR FLAME.

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 73

- **Hazardous Substances Data Bank (HSDB)**

11.1.8 Skin, Eye, and Respiratory Irritations

Immediately irritating to the eye. /Cyanides/

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS(NIOSH) Publication No. 90-117. Washington, DC: U.S. Government Printing Office, June 1990, p. 76

- **Hazardous Substances Data Bank (HSDB)**

... HUMAN SKIN EXPOSURES TO ADIPONITRILE RESULT IN SKIN IRRITATION ...

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3153

- Hazardous Substances Data Bank (HSDB)

11.2 Safety and Hazard Properties

11.2.1 Flammable Limits

LOWER 1.0% @ 200 °C

U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5.

- Hazardous Substances Data Bank (HSDB)

Flammability

Class IIIA Combustible Liquid: Fl.P. at or above 140 °F and below 200 °F.

- The National Institute for Occupational Safety and Health (NIOSH)

11.2.2 Lower Explosive Limit (LEL)

1 % at 392F (EPA, 1998)

U.S. Environmental Protection Agency. 1998. Extremely Hazardous Substances (EHS) Chemical Profiles and Emergency First Aid Guides. Washington, D.C.: U.S. Government Printing Office.

- CAMEO Chemicals

1.7%

- Occupational Safety and Health Administration (OSHA); The National Institute for Occupational S...

11.2.3 Upper Explosive Limit (UEL)

5 % (NIOSH, 2024)

- CAMEO Chemicals

5.0%

- Occupational Safety and Health Administration (OSHA); The National Institute for Occupational S...

11.2.4 Critical Temperature & Pressure

Critical temperature: 507 °C; Critical pressure: 2.8 MPa (27.6 atm)

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. SUPP (1998) 445

- Hazardous Substances Data Bank (HSDB)

11.2.5 Explosive Limits and Potential

Explosive limits , vol% in air: 1.7-4.9

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.2.6 NIOSH Recommendations

Recommended Exposure Limit: 10 Hr Time-Weighted Avg: 4 ppm (18 mg/cu m).

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 8

- Hazardous Substances Data Bank (HSDB)

11.3 First Aid Measures

Inhalation First Aid

Fresh air, rest. Administration of oxygen may be needed. No mouth-to-mouth artificial respiration. Refer immediately for medical attention.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Skin First Aid

Remove contaminated clothes. Rinse and then wash skin with water and soap. Administration of oxygen may be needed. Refer immediately for medical attention.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Eye First Aid

Rinse with plenty of water for several minutes (remove contact lenses if easily possible). Refer for medical attention.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Ingestion First Aid

Rinse mouth. Administration of oxygen may be needed. Give one or two glasses of water to drink. Refer for medical attention .

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.3.1 First Aid

Warning: Effects may be delayed. Caution is advised. Vital signs should be monitored closely.

Signs and Symptoms of Acute Adiponitrile Exposure: Signs and symptoms of acute exposure to adiponitrile may include tightness of the chest and tachypnea (rapid respiratory rate). Tachycardia (rapid heart rate), hypotension (low blood pressure), and cyanosis (blue tint to skin and mucous membranes) may also occur. Victims may experience headache, weakness, dizziness, difficulty in standing, dilated pupils, confusion, and seizures. Vomiting has been reported. Adiponitrile may irritate or burn the skin, eyes, and mucous membranes.

Emergency Life-Support Procedures: Acute exposure to adiponitrile may require decontamination and life support for the victims. All exposed persons should be transported to a health care facility as quickly as possible. Emergency personnel should wear protective clothing appropriate to the type and degree of contamination. Air-purifying or supplied-air respiratory equipment should also be worn, as necessary. Rescue vehicles should carry supplies such as plastic sheeting and disposable plastic bags to assist in preventing spread of contamination.

Inhalation Exposure:

1. Move victims to fresh air. Emergency personnel should avoid self-exposure to adiponitrile.

2. Evaluate vital signs including pulse and respiratory rate, and note any trauma. If no pulse is detected, provide CPR. If not breathing, provide artificial respiration. IMMEDIATELY begin administering 100% oxygen to all victims. Monitor victims for respiratory distress.Warning: To prevent self-poisoning, avoid mouth-to-mouth breathing; use a forced-oxygen mask. Direct oral contact with adiponitrile-contaminated persons or their gastric contents can result in self-poisoning.

3. RUSH to a health care facility!

4. Obtain authorization and/or further instructions from the local hospital for administration of an antidote or performance of other invasive procedures.

Dermal/Eye Exposure:

1. Remove victims from exposure. Emergency personnel should avoid self- exposure to adiponitrile.

2. Evaluate vital signs including pulse and respiratory rate, and note any trauma. If no pulse is detected, provide CPR. If not breathing, provide artificial respiration. IMMEDIATELY begin administering 100% **oxygen** to all victims. Monitor victims for respiratory distress.Warning: To prevent self-poisoning, avoid mouth-to-mouth breathing; use a forced-**oxygen** mask. Direct oral contact with adiponitrile-contaminated persons or their gastric contents can result in self-poisoning.

3. RUSH to a health care facility!

4. Remove contaminated clothing as soon as possible.

5. If eye exposure has occurred, eyes must be flushed with lukewarm **water** for at least 15 minutes.

6. Wash exposed skin areas twice with soap and **water**.

7. Obtain authorization and/or further instructions from the local hospital for administration of an antidote or performance of other invasive procedures.

Ingestion Exposure:

1. Evaluate vital signs including pulse and respiratory rate, and note any trauma. If no pulse is detected, provide CPR. If not breathing, provide artificial respiration. IMMEDIATELY begin administering 100% **oxygen** to all victims. Monitor victims for respiratory distress.Warning: To prevent self-poisoning, avoid mouth-to-mouth breathing; use a forced-**oxygen** mask. Direct oral contact with adiponitrile-contaminated persons or their gastric contents can result in self-poisoning.

2. RUSH to a health care facility!

3. DO NOT induce vomiting. Ipecac is not recommended for ingestion of adiponitrile.

4. Obtain authorization and/or further instructions from the local hospital for administration of an antidote or performance of other invasive procedures.

5. Activated **charcoal** may be administered if victims are conscious and alert. Use 15 to 30 g (1/2 to 1 oz) for children, 50 to 100 g (1-3/4 to 3-1/2 oz) for adults, with 125 to 250 mL (1/2 to 1 cup) of **water**.

6. Promote excretion by administering a saline cathartic or **sorbitol** to conscious and alert victims. Children require 15 to 30 g (1/2 to 1 oz) of cathartic; 50 to 100 g (1-3/4 to 3-1/2 oz) is recommended for adults. (EPA, 1998)

U.S. Environmental Protection Agency. 1998. Extremely Hazardous Substances (EHS) Chemical Profiles and Emergency First Aid Guides. Washington, D.C.: U.S. Government Printing Office.

- **CAMEO Chemicals**

ERG 2024, Guide 153 (Adiponitrile)

General First Aid:

· Call 911 or emergency medical service.

· Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and avoid contamination.

· Move victim to fresh air if it can be done safely.

· Administer oxygen if breathing is difficult.

· If victim is not breathing:

-- DO NOT perform mouth-to-mouth resuscitation; the victim may have ingestedor inhaled the substance.

-- If equipped and pulse detected, wash face and mouth, then give artificial respiration using a proper respiratory medical device (bag-valve mask, pocket mask equipped with a one-way valve or other device).

-- If no pulse detected or no respiratory medical device available, provide continuouscompressions. Conduct a pulse check every two minutes or monitor for any signs of spontaneous respirations.

· Remove and isolate contaminated clothing and shoes.

· For minor skin contact, avoid spreading material on unaffected skin.

· In case of contact with substance, remove immediately by flushing skin or eyes with running water for at least 20 minutes.

· For severe burns, immediate medical attention is required.

· Effects of exposure (inhalation, ingestion, or skin contact) to substance may be delayed.

· Keep victim calm and warm.

· Keep victim under observation.

· For further assistance, contact your local Poison Control Center.

· Note: Basic Life Support (BLS) and Advanced Life Support (ALS) should be done by trained professionals.

Specific First Aid:

· For corrosives, in case of contact, immediately flush skin or eyes with running water for at least 30 minutes. Additional flushing may be required.

· Removal of solidified molten material from skin requires medical assistance.

In Canada, an Emergency Response Assistance Plan (ERAP) may be required for this product. Please consult the shipping paper and/or the "ERAP" section.

- Emergency Response Guidebook (ERG)

(See general first aid procedures)

Eye: Irrigate immediately - If this chemical contacts the eyes, immediately wash (irrigate) the eyes with large amounts of **water**, occasionally lifting the lower and upper lids. Get medical attention immediately.

Skin: Soap wash immediately - If this chemical contacts the skin, immediately wash the contaminated skin with soap and **water**. If this chemical penetrates the clothing, immediately remove the clothing, wash the skin with soap and **water**, and get medical attention promptly.

Breathing: Respiratory support

Swallow: Medical attention immediately - If this chemical has been swallowed, get medical attention immediately.

- **The National Institute for Occupational Safety and Health (NIOSH)**

11.4 Fire Fighting

Wear chemical protective suit with self-contained breathing apparatus. Cool exposed containers with **water**.

Use dry chemical, **carbon dioxide**, **water** spray, fog or foam. (EPA, 1998)

U.S. Environmental Protection Agency. 1998. Extremely Hazardous Substances (EHS) Chemical Profiles and Emergency First Aid Guides. Washington, D.C.: U.S. Government Printing Office.

- **CAMEO Chemicals**

Use **water** spray, foam, powder, **carbon dioxide**. In case of fire: keep drums, etc., cool by spraying with **water**.

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

11.4.1 Fire Fighting Procedures

USE **WATER** SPRAY, DRY CHEMICAL, FOAM OR **CARBON DIOXIDE**. USE **WATER** SPRAY TO KEEP FIRE-EXPOSED CONTAINERS COOL. APPROACH FIRE FROM UPWIND TO AVOID HAZARDOUS VAPORS AND TOXIC DECOMPOSITION PRODUCTS.

Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 49-13

- **Hazardous Substances Data Bank (HSDB)**

If material on fire or involved in fire: Use **water** in flooding quantities as fog. use foam, dry chemical, or **carbon dioxide**. Keep run-off **water** out of sewers and **water** sources. Cool all

affected containers with flooding quantities of water. Apply water form as far a distance as possible.

Association of American Railroads. Emergency Handling of Hazardous Materials in Surface Transportation. Washington, DC: Association of American Railroads, Bureau of Explosives, 1994., p. 18

▸ Hazardous Substances Data Bank (HSDB)

11.5 Accidental Release Measures

Public Safety: ERG 2024, Guide 153 (Adiponitrile)

· CALL 911. Then call emergency response telephone number on shipping paper. If shipping paper not available or no answer, refer to appropriate telephone number listed on the inside back cover.

· Keep unauthorized personnel away.

· Stay upwind, uphill and/or upstream.

· Ventilate closed spaces before entering, but only if properly trained and equipped.

▸ Emergency Response Guidebook (ERG)

Spill or Leak: ERG 2024, Guide 153 (Adiponitrile)

· ELIMINATE all ignition sources (no smoking, flares, sparks or flames) from immediate area.

· Do not touch damaged containers or spilled material unless wearing appropriate protective clothing.

· Stop leak if you can do it without risk.

· Prevent entry into waterways, sewers, basements or confined areas.

· Absorb or cover with dry earth, sand or other non-combustible material and transfer to containers.

· DO NOT GET WATER INSIDE CONTAINERS.

▸ Emergency Response Guidebook (ERG)

11.5.1 Isolation and Evacuation

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]:

IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids.

SPILL: Increase the immediate precautionary measure distance, in the downwind direction, as necessary.

FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

2024 Emergency Response Guidebook, ***https://www.phmsa.dot.gov/training/hazmat/erg/emergency-response-guidebook-erg***

- CAMEO Chemicals

Evacuation: ERG 2024, Guide 153 (Adiponitrile)

Immediate precautionary measure

· Isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids.

Spill

· For highlighted materials: see Table 1 - Initial Isolation and Protective Action Distances.

· For non-highlighted materials: increase the immediate precautionary measure distance, in the downwind direction, as necessary.

Fire

· If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions.

- Emergency Response Guidebook (ERG)

11.5.2 Spillage Disposal

Personal protection: complete protective clothing including self-contained breathing apparatus. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.5.3 Cleanup Methods

Stop or control the leak, if this can be done without undue risk. Use **water** spray to cool and disperse vapors, and protect personnel. Approach release from upwind. Absorb in noncombustible material for proper disposal.

Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 49-13

- Hazardous Substances Data Bank (HSDB)

11.5.4 Disposal Methods

A poor candidate for incineration. /Cyanides/

USEPA; Engineering Handbook for Hazardous Waste Incineration p.3-8 (1981) EPA 68-03-3025

- Hazardous Substances Data Bank (HSDB)

11.5.5 Preventive Measures

The worker should immediately wash the skin when it becomes contaminated.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 8

- Hazardous Substances Data Bank (HSDB)

Work clothing that becomes wet or significantly contaminated should be removed oand replaced.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 8

- Hazardous Substances Data Bank (HSDB)

Workers whose clothing may have become contaminated should change into uncontaminated clothing before leaving the work premises.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 8

- Hazardous Substances Data Bank (HSDB)

SRP: Contaminated protective clothing should be segregated in such a manner so that there is no direct personal contact by personnel who handle, dispose, or clean the clothing. Quality assurance to ascertain the completeness of the cleaning procedures should be implemented before the decontaminated protective clothing is returned for reuse by the workers. Contaminated clothing should not be taken home at end of shift, but should remain at employee's place of work for cleaning.

- Hazardous Substances Data Bank (HSDB)

For more Preventive Measures (Complete) data for ADIPONITRILE (9 total), please visit the HSDB record page.

- Hazardous Substances Data Bank (HSDB)

11.6 Handling and Storage

11.6.1 Nonfire Spill Response

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]:

ELIMINATE all ignition sources (no smoking, flares, sparks or flames) from immediate area. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Stop leak if you can do it without risk. Prevent entry into waterways, sewers, basements or confined areas. Absorb or cover with dry earth, sand or other non-combustible material and transfer to containers. DO NOT GET WATER INSIDE CONTAINERS. (ERG, 2024)

*2024 Emergency Response Guidebook, **https://www.phmsa.dot.gov/training/hazmat/erg/emergency-response-guidebook-erg***

- CAMEO Chemicals

11.6.2 Safe Storage

Separated from strong oxidants, strong acids and food and feedstuffs. Ventilation along the floor.

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.6.3 Storage Conditions

Separate from strong acids and oxidizing materials. Store in a cool, dry, well-ventilated location. Outside or detached storage is preferred.

Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 49-13

- Hazardous Substances Data Bank (HSDB)

11.7 Exposure Control and Personal Protection

Protective Clothing: ERG 2024, Guide 153 (Adiponitrile)

· Wear positive pressure self-contained breathing apparatus (SCBA).

· Wear chemical protective clothing that is specifically recommended by the manufacturer when there is NO RISK OF FIRE.

· Structural firefighters' protective clothing provides thermal protection but only limited chemical protection.

- Emergency Response Guidebook (ERG)

11.7.1 Recommended Exposure Limit (REL)

REL-TWA (Time Weighted Average)

4 ppm (18 mg/m^3)

- Occupational Safety and Health Administration (OSHA)

TWA 4 ppm (18 mg/m^3)

- The National Institute for Occupational Safety and Health (NIOSH)

11.7.2 Permissible Exposure Limit (PEL)

none

- The National Institute for Occupational Safety and Health (NIOSH)

11.7.3 Immediately Dangerous to Life or Health (IDLH)

N.D.

See: IDLH INDEX

- The National Institute for Occupational Safety and Health (NIOSH)

11.7.4 Threshold Limit Values (TLV)

2.0 [ppm]

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

8 hr Time Weighted Avg (TWA): 2 ppm, skin.

American Conference of Governmental Industrial Hygienists TLVs and BEIs. Threshold Limit Values for Chemical Substances and Physical Agents and Biological Exposure Indices. Cincinnati, OH, 2008, p. 11

- **Hazardous Substances Data Bank (HSDB)**

Excursion Limit Recommendation: Excursions in worker exposure levels may exceed 3 times the TLV-TWA for no more than a total of 30 minutes during a work day, and under no circumstances should they exceed 5 times the TLV-TWA, provided that the TLV-TWA is not exceeded.

American Conference of Governmental Industrial Hygienists TLVs and BEIs. Threshold Limit Values for Chemical Substances and Physical Agents and Biological Exposure Indices. Cincinnati, OH, 2008, p. 5

- **Hazardous Substances Data Bank (HSDB)**

2 ppm as TWA; (skin)

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

TLV-TWA (Time Weighted Average)

2 ppm [1990]

- **Occupational Safety and Health Administration (OSHA)**

11.7.5 Emergency Response Planning Guidelines

Emergency Response: ERG 2024, Guide 153 (Adiponitrile)

Small Fire

· Dry chemical, CO2 or **water** spray.

Large Fire

· Dry chemical, CO2, alcohol-resistant foam or **water** spray.

· If it can be done safely, move undamaged containers away from the area around the fire.

· Dike runoff from fire control for later disposal.

Fire Involving Tanks, Rail Tank Cars or Highway Tanks

· Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles.

· Do not get **water** inside containers.

· Cool containers with flooding quantities of **water** until well after fire is out.

· Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank.

· ALWAYS stay away from tanks in direct contact with flames.

- Emergency Response Guidebook (ERG)

11.7.6 Inhalation Risk

A harmful contamination of the air will not or will only very slowly be reached on evaporation of this substance at 20 °C.

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.7.7 Effects of Short Term Exposure

The substance is irritating to the eyes and skin. Exposure could cause convulsions, unconsciousness and death. Medical observation is indicated.

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.7.8 Effects of Long Term Exposure

The substance may have effects on the blood and adrenals. This may result in anaemia and tissue lesions.

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.7.9 Personal Protective Equipment (PPE)

Excerpt from NIOSH Pocket Guide for Adiponitrile:

Skin: PREVENT SKIN CONTACT - Wear appropriate personal protective clothing to prevent skin contact.

Eyes: PREVENT EYE CONTACT - Wear appropriate eye protection to prevent eye contact.

Wash skin: WHEN CONTAMINATED - The worker should immediately wash the skin when it becomes contaminated.

Remove: WHEN WET OR CONTAMINATED - Work clothing that becomes wet or significantly contaminated should be removed and replaced.

Change: DAILY - Workers whose clothing may have become contaminated should change into uncontaminated clothing before leaving the work premises. (NIOSH, 2024)

- CAMEO Chemicals

RUBBER GLOVES & CLOTHING GIVING FULL BODY & FACE PROTECTION TO AVOID CONTACT WITH SKIN. AIR OR OXYGEN MASK.

U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5.

- **Hazardous Substances Data Bank (HSDB)**

Wear appropriate personal protective clothing to prevent skin contact.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 8

- **Hazardous Substances Data Bank (HSDB)**

Wear appropriate eye protection to prevent eye contact.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 8

- **Hazardous Substances Data Bank (HSDB)**

Recommendations for respirator selection. Max concn for use: 40 ppm. Respirator Class(es): Any supplied-air respirator.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 8

- **Hazardous Substances Data Bank (HSDB)**

For more Personal Protective Equipment (PPE) (Complete) data for ADIPONITRILE (9 total), please visit the **HSDB record page**.

- **Hazardous Substances Data Bank (HSDB)**

(**See personal protection and sanitation codes**)

Skin: Prevent skin contact - Wear appropriate personal protective clothing to prevent skin contact.

Eyes: Prevent eye contact - Wear appropriate eye protection to prevent eye contact.

Wash skin: When contaminated

Remove: When wet or contaminated

Change: Daily - Workers whose clothing may have become contaminated should change into uncontaminated clothing before leaving the work premises.

- **The National Institute for Occupational Safety and Health (NIOSH)**

11.7.10 Respirator Recommendations

NIOSH

Up to 40 ppm:

(APF = 10) Any supplied-air respirator

Up to 100 ppm:

(APF = 25) Any supplied-air respirator operated in a continuous-flow mode

Up to 200 ppm:

(APF = 50) Any self-contained breathing apparatus with a full facepiece

(APF = 50) Any supplied-air respirator with a full facepiece

Up to 250 ppm:

(APF = 2000) Any supplied-air respirator that has a full facepiece and is operated in a pressure-demand or other positive-pressure mode

Emergency or planned entry into unknown concentrations or IDLH conditions:

(APF = 10,000) Any self-contained breathing apparatus that has a full facepiece and is operated in a pressure-demand or other positive-pressure mode

(APF = 10,000) Any supplied-air respirator that has a full facepiece and is operated in a pressure-demand or other positive-pressure mode in combination with an auxiliary self-contained positive-pressure breathing apparatus

Escape:

(APF = 50) Any air-purifying, full-facepiece respirator (gas mask) with a chin-style, front- or back-mounted organic vapor canister

Any appropriate escape-type, self-contained breathing apparatus

Important additional information about respirator selection

- **The National Institute for Occupational Safety and Health (NIOSH)**

11.7.11 Preventions

Fire Prevention

NO open flames.

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

Exposure Prevention

STRICT HYGIENE! IN ALL CASES CONSULT A DOCTOR!

- ILO-WHO International Chemical Safety Cards (ICSCs)

Inhalation Prevention

Use ventilation, local exhaust or breathing protection.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Skin Prevention

Protective gloves. Protective clothing.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Eye Prevention

Wear face shield.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Ingestion Prevention

Do not eat, drink, or smoke during work. Wash hands before eating.

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.8 Stability and Reactivity

11.8.1 Air and Water Reactions

No rapid reaction with air. No rapid reaction with water.

- CAMEO Chemicals

11.8.2 Reactive Group

Nitriles

- CAMEO Chemicals

11.8.3 Reactivity Profile

ADIPONITRILE is incompatible with strong oxidizers. It is also incompatible with strong acids, strong bases and strong reducing agents. (NTP, 1992).

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

- CAMEO Chemicals

11.8.4 Hazardous Reactivities and Incompatibilities

Oxidizers (e,g., perchlorates, nitrates), strong acids (e.g., **sulfuric acid**) [Note: Decomposes above 194 degrees F, forming **hydrogen cyanide**].

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 8

- Hazardous Substances Data Bank (HSDB)

... 18 Month old bottles of **iminodipropionitrile** exploded, probably owing to slow hydrolysis and release of **ammonia**.

Bretherick, L. Handbook of Reactive Chemical Hazards. 4th ed. Boston, MA: Butterworth-Heinemann Ltd., 1990, p. 636

- Hazardous Substances Data Bank (HSDB)

11.9 Transport Information

11.9.1 DOT Emergency Guidelines

/GUIDE 153: SUBSTANCES - TOXIC and/or CORROSIVE (Combustible)/ Fire or Explosion: Combustible material: may burn but does not ignite readily. When heated, vapors may form explosive mixtures with air: indoors, outdoors and sewers explosion hazards. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Contact with metals may evolve flammable **hydrogen** gas. Containers may explode when heated. Runoff may pollute waterways. Substance may be transported in a molten form.

U.S. Department of Transportation. 2012 Emergency Response Guidebook. Washington, D.C. 2012

- Hazardous Substances Data Bank (HSDB)

/GUIDE 153: SUBSTANCES - TOXIC and/or CORROSIVE (Combustible)/ Health: TOXIC; inhalation, ingestion or skin contact with material may cause severe injury or death. Contact with molten substance may cause severe burns to skin and eyes. Avoid any skin contact. Effects of contact or inhalation may be delayed. Fire may produce irritating, corrosive and/or toxic

gases. Runoff from fire control or dilution water may be corrosive and/or toxic and cause pollution.

U.S. Department of Transportation. 2012 Emergency Response Guidebook. Washington, D.C. 2012

- **Hazardous Substances Data Bank (HSDB)**

/GUIDE 153: SUBSTANCES - TOXIC and/or CORROSIVE (Combustible)/ Public Safety: CALL Emergency Response Telephone Number on Shipping Paper first. If Shipping Paper not available or no answer, refer to appropriate telephone number listed on the inside back cover. As an immediate precautionary measure, isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids. Keep unauthorized personnel away. Stay upwind. Keep out of low areas. Ventilate enclosed areas.

U.S. Department of Transportation. 2012 Emergency Response Guidebook. Washington, D.C. 2012

- **Hazardous Substances Data Bank (HSDB)**

/GUIDE 153: SUBSTANCES - TOXIC and/or CORROSIVE (Combustible)/ Protective Clothing: Wear positive pressure self-contained breathing apparatus (SCBA). Wear chemical protective clothing that is specifically recommended by the manufacturer. It may provide little or no thermal protection. Structural firefighters' protective clothing provides limited protection in fire situations ONLY; it is not effective in spill situations where direct contact with the substance is possible.

U.S. Department of Transportation. 2012 Emergency Response Guidebook. Washington, D.C. 2012

- **Hazardous Substances Data Bank (HSDB)**

For more DOT Emergency Guidelines (Complete) data for ADIPONITRILE (8 total), please visit the HSDB record page.

- **Hazardous Substances Data Bank (HSDB)**

11.9.2 DOT ID and Guide

2205 153

- **The National Institute for Occupational Safety and Health (NIOSH)**

11.9.3 Shipping Name / Number DOT/UN/NA/IMO

UN 2205; Adiponitrile

- Hazardous Substances Data Bank (HSDB)

IMO 6.1; Adiponitrile

- Hazardous Substances Data Bank (HSDB)

11.9.4 Shipment Methods and Regulations

No person may /transport,/ offer or accept a hazardous material for transportation in commerce unless that person is registered in conformance ... and the hazardous material is properly classed, described, packaged, marked, labeled, and in condition for shipment as required or authorized by ... /the hazardous materials regulations (49 CFR 171-177)./

49 CFR 171.2; U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of February 15, 2006: ***https://www.ecfr.gov***

- Hazardous Substances Data Bank (HSDB)

The International Air Transport Association (IATA) Dangerous Goods Regulations are published by the IATA Dangerous Goods Board pursuant to IATA Resolutions 618 and 619 and constitute a manual of industry carrier regulations to be followed by all IATA Member airlines when transporting hazardous materials.

International Air Transport Association. Dangerous Goods Regulations. 47th Edition. Montreal, Quebec Canada. 2006., p. 133

- Hazardous Substances Data Bank (HSDB)

The International Maritime Dangerous Goods Code lays down basic principles for transporting hazardous chemicals. Detailed recommendations for individual substances and a number of recommendations for good practice are included in the classes dealing with such substances. A general index of technical names has also been compiled. This index should always be consulted when attempting to locate the appropriate procedures to be used when shipping any substance or article.

International Maritime Organization. International Maritime Dangerous Goods Code. London, UK. 2004., p. 102

- Hazardous Substances Data Bank (HSDB)

11.9.5 DOT Label

Poison

- CAMEO Chemicals

11.9.6 Packaging and Labelling

Do not transport with food and feedstuffs.

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.9.7 UN Classification

UN Hazard Class: 6.1; UN Pack Group: III

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.10 Regulatory Information

The Australian Inventory of Industrial Chemicals

Chemical: Hexanedinitrile

- Australian Industrial Chemicals Introduction Scheme (AICIS)

REACH Registered Substance

Status: Active Update: 12-05-2022 https://echa.europa.eu/registration-dossier/-/registered-dossier/14296

- European Chemicals Agency (ECHA)

New Zealand EPA Inventory of Chemical Status

Adiponitrile: Does not have an individual approval but may be used under an appropriate group standard

- New Zealand Environmental Protection Authority (EPA)

11.10.1 Atmospheric Standards

This action promulgates standards of performance for equipment leaks of Volatile Organic Compounds (VOC) in the Synthetic Organic Chemical Manufacturing Industry (SOCMI). The intended effect of these standards is to require all newly constructed, modified, and reconstructed SOCMI process units to use the best demonstrated system of continuous

emission reduction for equipment leaks of VOC, considering costs, non air quality health and environmental impact and energy requirements. Adiponitrile is produced, as an intermediate or a final product, by process units covered under this subpart.

40 CFR 60.489 (7/1/2000)

- **Hazardous Substances Data Bank (HSDB)**

11.10.2 CERCLA Reportable Quantities

Releases of CERCLA hazardous substances are subject to the release reporting requirement of CERCLA section 103, codified at 40 CFR part 302, in addition to the requirements of 40 CFR part 355. Adiponitrile is an extremely hazardous substance (EHS) subject to reporting requirements when stored in amounts in excess of its threshold planning quantity (TPQ) of 1000 lbs.

40 CFR 355 (7/1/2000)

- **Hazardous Substances Data Bank (HSDB)**

11.10.3 TSCA Requirements

Pursuant to section 8(d) of **TSCA**, EPA promulgated a model Health and Safety Data Reporting Rule. The section 8(d) model rule requires manufacturers, importers, and processors of listed chemical substances and mixtures to submit to EPA copies and lists of unpublished health and safety studies. **Hexanedinitrile** is included on this list.

40 CFR 716.120 (7/1/2000)

- **Hazardous Substances Data Bank (HSDB)**

11.11 Other Safety Information

11.11.1 Toxic Combustion Products

Products of combustion may be more hazardous than the material itself. By-products include **hydrogen cyanide** and irritants.

Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 49-13

- **Hazardous Substances Data Bank (HSDB)**

11.11.2 Special Reports

Kaplita PV and Smith RP; Toxicol Appl Pharmacol 84 (3): 533-540 (1986). Pathways for the bioactivation of aliphatic nitriles to free **cyanide** in mice.

- **Hazardous Substances Data Bank (HSDB)**

Homan ER; Clinical and Experimental Toxicol of Cyanides, Bristol, UK 1-21 pages (1987). Reactions, industrial processes, and materials with potential for exposure to **cyanide** compounds were discussed in this overview on the toxicology of cyanides.

- **Hazardous Substances Data Bank (HSDB)**

12 Toxicity

12.1 Toxicological Information

12.1.1 Toxicity Summary

Organic nitriles decompose into **cyanide** ions both in vivo and in vitro. Consequently the primary mechanism of toxicity for organic nitriles is their production of toxic **cyanide** ions or **hydrogen cyanide**. **Cyanide** is an inhibitor of cytochrome c oxidase in the fourth complex of the electron transport chain (found in the membrane of the mitochondria of eukaryotic cells). It complexes with the **ferric iron** atom in this enzyme. The binding of **cyanide** to this cytochrome prevents transport of electrons from cytochrome c oxidase to **oxygen**. As a result, the electron transport chain is disrupted and the cell can no longer aerobically produce **ATP** for energy. Tissues that mainly depend on aerobic respiration, such as the central nervous system and the heart, are particularly affected. **Cyanide** is also known produce some of its toxic effects by binding to catalase, **glutathione** peroxidase, methemoglobin, **hydroxocobalamin**, phosphatase, tyrosinase, **ascorbic acid** oxidase, **xanthine** oxidase, succinic dehydrogenase, and Cu/Zn superoxide dismutase. **Cyanide** binds to the **ferric** ion of methemoglobin to form inactive cyanmethemoglobin. (L97)

L97: Wikipedia. Cyanide poisoning. Last Updated 30 March 2009.
http://en.wikipedia.org/wiki/Cyanide_poisoning

- **Toxin and Toxin Target Database (T3DB)**

12.1.2 EPA IRIS Information

Substance	Adiponitrile
Toxicity Summary	EPA IRIS Summary PDF (Update: Feb-01-1991)

- EPA Integrated Risk Information System (IRIS)

12.1.3 EPA Provisional Peer-Reviewed Toxicity Values

Chemical Substance	Adiponitrile
Reference Concentration (RfC), Chronic	6 x 10^-3 mg/m^3
Reference Concentration (RfC), Subchronic	6 x 10^-2 mg/m^3
PPRTV Assessment	PDF Document
Weight-Of-Evidence (WOE)	Inadequate information to assess carcinogenic potential
Last Revision	2005

- EPA Provisional Peer-Reviewed Toxicity Values (PPRTVs)

12.1.4 RAIS Toxicity Values

Inhalation Chronic Reference Concentration (RfC) (mg/m^3)	0.006
Inhalation Chronic Reference Concentration Reference	PPRTV Current
Inhalation Subchronic Reference Concentration (RfCs) (mg/m^3)	0.06
Inhalation Subchronic Reference Concentration Reference	PPRTV Current

- Risk Assessment Information System (RAIS)

12.1.5 NIOSH Toxicity Data

- The National Institute for Occupational Safety and Health (NIOSH)

12.1.6 Evidence for Carcinogenicity

CLASSIFICATION: D; not classifiable as to human carcinogenicity. BASIS FOR CLASSIFICATION: No human and no animal cancer data were available. Adiponitrile was negative for mutagenicity in Salmonella with and without activation. HUMAN CARCINOGENICITY DATA: None. ANIMAL CARCINOGENICITY DATA: None.

U.S. Environmental Protection Agency's Integrated Risk Information System (IRIS). Summary on Adiponitrile (111-69-3). Available from, as of March 15, 2000: ***https://www.epa.gov/iris/***

- Hazardous Substances Data Bank (HSDB)

12.1.7 Carcinogen Classification

Carcinogen Classification	No indication of carcinogenicity to humans (not listed by IARC).

- Toxin and Toxin Target Database (T3DB)

12.1.8 Health Effects

Exposure to high levels of cyanide for a short time harms the brain and heart and can even cause coma, seizures, apnea, cardiac arrest and death. Chronic inhalation of cyanide causes breathing difficulties, chest pain, vomiting, blood changes, headaches, and enlargement of the thyroid gland. Skin contact with cyanide salts can irritate and produce sores. (L96, L97)

L96: ATSDR - Agency for Toxic Substances and Disease Registry (2006). Toxicological profile for cyanide. U.S. Public Health Service in collaboration with U.S. Environmental Protection Agency (EPA).
http://www.atsdr.cdc.gov/toxprofiles/tp8.html

L97: Wikipedia. Cyanide poisoning. Last Updated 30 March 2009.
http://en.wikipedia.org/wiki/Cyanide_poisoning

- **Toxin and Toxin Target Database (T3DB)**

12.1.9 Exposure Routes

The substance can be absorbed into the body by inhalation, through the skin and by ingestion.

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

inhalation, skin absorption, ingestion, skin and/or eye contact

- **The National Institute for Occupational Safety and Health (NIOSH)**

Oral (L96) ; inhalation (L96) ; dermal (L96)

L96: ATSDR - Agency for Toxic Substances and Disease Registry (2006). Toxicological profile for cyanide. U.S. Public Health Service in collaboration with U.S. Environmental Protection Agency (EPA).
http://www.atsdr.cdc.gov/toxprofiles/tp8.html

- **Toxin and Toxin Target Database (T3DB)**

12.1.10 Symptoms

Inhalation Exposure

Headache. Vomiting. Dizziness. Nausea. Laboured breathing. Confusion. Convulsions.

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

Skin Exposure

MAY BE ABSORBED! Redness. Pain.

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

Eye Exposure

Redness. Blurred vision.

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

Ingestion Exposure

Abdominal pain. Further see Inhalation.

- ILO-WHO International Chemical Safety Cards (ICSCs)

irritation eyes, skin, respiratory system; headache, dizziness, lassitude (weakness, exhaustion), confusion, convulsions; blurred vision; dyspnea (breathing difficulty); abdominal pain, nausea, vomiting

- The National Institute for Occupational Safety and Health (NIOSH)

Cyanide poisoning is identified by rapid, deep breathing and shortness of breath, general weakness, giddiness, headaches, vertigo, confusion, convulsions/seizures and eventually loss of consciousness. (L96, L97)

L96: ATSDR - Agency for Toxic Substances and Disease Registry (2006). Toxicological profile for cyanide. U.S. Public Health Service in collaboration with U.S. Environmental Protection Agency (EPA). ***http://www.atsdr.cdc.gov/toxprofiles/tp8.html***

L97: Wikipedia. Cyanide poisoning. Last Updated 30 March 2009. ***http://en.wikipedia.org/wiki/Cyanide_poisoning***

- Toxin and Toxin Target Database (T3DB)

12.1.11 Target Organs

Eyes, skin, respiratory system, central nervous system, cardiovascular system

- The National Institute for Occupational Safety and Health (NIOSH)

12.1.12 Adverse Effects

Other Poison - Chemical Asphyxiant

Dermatotoxin - Skin burns.

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

12.1.13 Acute Effects

- ChemIDplus

12.1.14 Toxicity Data

LC50 (rat) = 1,710 mg/m3/4h

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

LD50: 155 mg/kg (Oral, Rat) (T14) LD50: 40 mg/kg (Intraperitoneal, Mouse) (T14) LD50: 50 mg/kg (Subcutaneous, Guinea pig) (T32) LC50: 1.71 mg/L over 4 hours (Inhalation, Rat) (T88)

T14: Lewis RJ (1996). Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold.

T32: Verschueren K (1983). Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co.

T88: Snyder, R (1990). Ethyl Browning's Toxicity and Metabolism of Industrial Solvents. 2nd ed. Volume II: Nitrogen and Phosphorus Solvents. Amsterdam-New York-Oxford: Elsevier.

- Toxin and Toxin Target Database (T3DB)

12.1.15 Treatment

Antidotes to **cyanide** poisoning include **hydroxocobalamin** and **sodium nitrite**, which release the **cyanide** from the cytochrome system, and rhodanase, which is an enzyme occurring naturally in mammals that combines serum **cyanide** with **thiosulfate**, producing comparatively harmless **thiocyanate**. **Oxygen** therapy can also be administered. (L97)

L97: Wikipedia. Cyanide poisoning. Last Updated 30 March 2009.
http://en.wikipedia.org/wiki/Cyanide_poisoning

- Toxin and Toxin Target Database (T3DB)

12.1.16 Interactions

The toxic mechanism of nitriles (including adiponitrile) and the effect of metabolic modifiers in mice were studied in relation to their physicochemical properties. All the test nitriles liberated **cyanide** both in vivo and in vitro, with the exception of **benzonitrile**, although the extent of liberation and the effect of **carbon tetrachloride** pretreatment on the mortality of animals differed among nitriles. From these results, test compounds were tentatively divided into 3 groups. In group 1, acute toxicity was greatly reduced by **carbon tetrachloride** pretreatment, in group 2, toxicity was not significantly changed or was somewhat enhanced, and in group 3, **benzonitrile** only, toxicity was clearly enhanced. The amount of **cyanide** was higher at death in the brains of mice given group 1 compounds, the level being comparable to that found in mice killed by dosing with **potassium cyanide**. The relation between log (1/LD50) and log p for the compounds in group 1 fitted a parabolic plot, while that for compounds in group 2 was linear. For most nitriles, the in vitro metabolism was inhibited when the incubation mixture contained either **SKF-525A**, **carbon monoxide**, or microsomes from mice treated with **carbon tetrachloride**. When mice were closed with **ethyl alcohol**, metabolic enhancement of nitriles was seen compared with the control. However, **ethyl alcohol**, when added to the incubation mixture, inhibited the in vitro metabolism of nitriles.

Tanii H; Juzen Igakkai Zasshi 94 (4): 664-77 (1985)

- **Hazardous Substances Data Bank (HSDB)**

12.1.17 Antidote and Emergency Treatment

A person who has inhaled the vapors should be moved to an uncontaminated environment, and cardiopulmonary resuscitation should be administered. If the victim breathes with difficulty, **oxygen** should be given. In case of eye contact, flush with copious **water** for at least 20 min and call a physician. In case of ingestion, induce vomiting and call a physician. For skin contact, wash with plenty of soap and **water**.

Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984., p. V15 900 (1981)

- **Hazardous Substances Data Bank (HSDB)**

Rapid support of respiration & circulation is essential to successful treatment of **cyanide** intoxication. Massive **cyanide** overdoses have survived with only good supportive care. Immediate attention should be directed toward assisted ventilation, admin of 100% **oxygen**, insertion of iv lines, & institution of cardiac monitoring. Obtain an arterial blood gas immediately & correct any severe metabolic acidosis (pH below 7.15). **Oxygen** (100%) should be used routinely in moderate or severely symptomatic patients even in the presence of a

normal pO2, since 100% O2 incr O2 delivery, may reactivate **cyanide**-inhibited mitochondrial enzymes, & potentiates the effect of **thiosulfate**. Avoid mouth to mouth resuscitation during CPR in order to prevent self poisoning. /Cyanides/

Ellenhorn, M.J., S. Schonwald, G. Ordog, J. Wasserberger. Ellenhorn's Medical Toxicology: Diagnosis and Treatment of Human Poisoning. 2nd ed. Baltimore, MD: Williams and Wilkins, 1997., p. 1480

Hazardous Substances Data Bank (HSDB)

Amyl nitrite perles are designed to produce 3% to 5% methemoglobinemia while an iv line is established for iv **sodium nitrite**. As a temporizing measure, the patient inhales the vapors until the **sodium nitrite** is ready. Because of the variability in methemoglobin production & the potential for cardiovascular collapse, this step may be omitted if **sodium nitrite** is readily available & the patient is not in extremis. Adequate ventilation & oxygenation are more important than admin of **amyl nitrite**. One perle (0.2 ml) is crushed & inhaled for 30 sec every min until iv **nitrite** is given. **Sodium nitrite** (3% soln), as 10 ml of a 3% soln (eg, 300 mg), is admin iv slowly over 4 min to produce a 20% methemoglobin level in adults. Children should receive 0.33 ml of the 3% soln/kg initially at an infusion rate of 2.5 ml/min, up to a maximum of 10 ml. Administer **sodium nitrite** doses to children on the basis of body weight, since fatal methemoglobinemia has occurred in children. /Cyanides/

Ellenhorn, M.J., S. Schonwald, G. Ordog, J. Wasserberger. Ellenhorn's Medical Toxicology: Diagnosis and Treatment of Human Poisoning. 2nd ed. Baltimore, MD: Williams and Wilkins, 1997., p. 1481

Hazardous Substances Data Bank (HSDB)

Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilation if necessary. Administer **oxygen** by nonrebreather mask at 10 to 15 L/min. Administer **amyl nitrite** ampules as per protocol and physician order ... . Monitor for shock and treat if necessary ... . Monitor for pulmonary edema and treat if necessary ... . Anticipate seizures and treat if necessary ... . For eye contamination, flush eyes immediately with **water**. Irrigate each eye continuously with **normal saline** during transport ... . Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of **water** for dilution if the patient can swallow, has a strong gag reflex, and does not drool ... . /**Cyanide** and related compounds/

Bronstein, A.C., P.L. Currance; Emergency Care for Hazardous Materials Exposure. 2nd ed. St. Louis, MO. Mosby Lifeline. 1994., p. 388

Hazardous Substances Data Bank (HSDB)

For more Antidote and Emergency Treatment (Complete) data for ADIPONITRILE (6 total), please visit the **HSDB record page**.

- Hazardous Substances Data Bank (HSDB)

12.1.18 Human Toxicity Excerpts

A case history of human exposure ... reported the effects of drinking "a few milliliters" of adiponitrile by an 18 yr old male. About 20 min after ingestion he experienced tightness in the chest, headache, weakness with difficulty in standing, and vertigo. He became cyanotic, respirations were rapid, & he had low blood pressure & tachycardia. The pupils were dilated & barely reacted to light. He exhibited mental confusion & tonic-clonic contractions of limbs & facial muscles.

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3152-3

- Hazardous Substances Data Bank (HSDB)

... Human skin exposure to adiponitrile result in skin irritation and inflammation ... one case in which adiponitrile caused massive destruction of the skin on one foot.

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3153

- Hazardous Substances Data Bank (HSDB)

HIGHLY TOXIC BY INGESTION, INHALATION & SKIN ABSORPTION. IT PRODUCES DISTURBANCES OF RESPIRATORY & CIRCULATORY SYSTEMS.

National Fire Protection Guide. Fire Protection Guide on Hazardous Materials. 10 th ed. Quincy, MA: National Fire Protection Association, 1991., p. 49-20

- Hazardous Substances Data Bank (HSDB)

POISONING BY ADIPONITRILE RESEMBLES POISONING WITH **HYDROCYANIC ACID** ... .

Lefaux, R. Practical Toxicology of Plastics. Cleveland: CRC Press Inc., 1968., p. 108

- Hazardous Substances Data Bank (HSDB)

For more Human Toxicity Excerpts (Complete) data for ADIPONITRILE (6 total), please visit the **HSDB record page**.

- Hazardous Substances Data Bank (HSDB)

12.1.19 Non-Human Toxicity Excerpts

A 2 yr drinking water exposure of Wistar rats at 0.5, 5.0, & 50 ppm adiponitrile produced significant adrenal degeneration in female rats at all 3 conc & at 50 ppm in male rats. All body wt & organ wt ratios of spleen, liver, & kidney were within normal ranges.

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3152

Hazardous Substances Data Bank (HSDB)

Exposures of pregnant Sprague Dawley rats at 10, 100, & 500 ppm in drinking water did not change ... gestation, or viability of offspring. Exposure of mongrel dogs to approx 10, 100, 500, & 1000 ppm adiponitrile in the diet resulted in greatly decr food intake & vomiting at 1000 ppm. No hematologic abnormalities were found. Kidney & liver function were normal at 500 ppm & below.

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3152

Hazardous Substances Data Bank (HSDB)

MEDIAN LETHAL CONCN WAS 1.71 MG/L FOR ACUTE (4 HR) INHALATION OF ADULT MALE CHR-CD RATS. RATS WERE EXPOSED TO 0 (CONTROL), 0.03, 0.1 OR 0.3 MG VAPORIZED ADIPONITRILE/L FOR 10 6-HR PERIODS (5 EXPOSURE DAYS, 2 REST DAYS, 5 EXPOSURE DAYS). CLINICAL SIGNS DURING EXPOSURE INCL IRREGULAR RESPIRATION & MILD SALIVATION. AT 0.3 MG/L RATS SHOWED WT LOSS DURING 1ST 5 EXPOSURES FOLLOWED BY NORMAL RATE OF WT GAIN. AFTER 10 EXPOSURES, RATS IN THIS GROUP SHOWED INCR BLOOD GLUCOSE, UREA NITROGEN, CREATININE & URINE GLUCOSE; DECR ERYTHROCYTES COUNT, HEMOGLOBIN, LEUKOCYTE COUNT, RELATIVE NUMBER OF EOSINOPHILS, & URINE OSMOLALITY. RATS EXPOSED TO 0.1 MG/L HAD INCR UREA NITROGEN & LYMPHOCYTES & DECR NUMBER OF NEUTROPHILS & EOSINOPHILS. RATS FROM ALL GROUPS HAD NORMAL VALUES 14 DAYS AFTER LAST EXPOSURE.

PMID:7179283

SMITH LW, KENNEDY GL JR; TOXICOL APPL PHARMACOL 65 (2): 257 (1982)

Hazardous Substances Data Bank (HSDB)

Adiponitrile was evaluated for embryotoxic and teratogenic potential in rats. Mated Sprague Dawley rats were administered adiponitrile by gavage on gestation days 6-19, inclusive. Daily dosage levels (mg/kg body wt) were 0, 20, 40, and 80. There was evidence of maternal toxicity in the high dose group. Some maternal effects also were seen at the middle dosage. Slight fetotoxicity was observed at the highest dosage. No teratogenic effects were observed at any dosage level.

PMID:3732670

Johannsen FR et al; Fundam Appl Toxicol 7 (1): 33-40 (1986)

- **Hazardous Substances Data Bank (HSDB)**

For more Non-Human Toxicity Excerpts (Complete) data for ADIPONITRILE (7 total), please visit the **HSDB record page**.

- **Hazardous Substances Data Bank (HSDB)**

12.1.20 Non-Human Toxicity Values

LD50 Guinea pig sc 50 mg/kg

Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983., p. 166

- **Hazardous Substances Data Bank (HSDB)**

LD50 Rat oral 155 mg/kg

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 73

- **Hazardous Substances Data Bank (HSDB)**

LD50 Mouse ip 40 mg/kg

Snyder, R. (ed.). Ethel Browning's Toxicity and Metabolism of Industrial Solvents. 2nd ed. Volume II: Nitrogen and Phosphorus Solvents. Amsterdam-New York-Oxford: Elsevier, 1990., p. 326

- **Hazardous Substances Data Bank (HSDB)**

LC50 Rat inhalation 1.71 mg/l/4 hr

Snyder, R. (ed.). Ethel Browning's Toxicity and Metabolism of Industrial Solvents. 2nd ed. Volume II: Nitrogen and Phosphorus Solvents. Amsterdam-New York-Oxford: Elsevier, 1990., p. 326

- **Hazardous Substances Data Bank (HSDB)**

For more Non-Human Toxicity Values (Complete) data for ADIPONITRILE (6 total), please visit the **HSDB record page**.

- **Hazardous Substances Data Bank (HSDB)**

12.2 Ecological Information

12.2.1 Ecotoxicity Values

TLm Pimephales promelas (fathead minnow) 820 mg/l/96 hr (hard water) /Conditions of bioassay not specified/

Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983., p. 166

- Hazardous Substances Data Bank (HSDB)

TLm Pimephales promelas (fathead minnow) 1250 mg/l/96 hr (soft water) /Conditions o bioassay not specified/

Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983., p. 166

- Hazardous Substances Data Bank (HSDB)

TLm Bluegill sunfish 1250 mg/l/24 hr (soft water) /Conditions of bioassay not specified/

Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983., p. 166

- Hazardous Substances Data Bank (HSDB)

TLm Guppies 775 mg/l/96 hr (soft water) /Conditions of bioassay not specified/

Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983., p. 166

- Hazardous Substances Data Bank (HSDB)

12.2.2 US EPA Regional Screening Levels for Chemical Contaminants

Resident Soil (mg/kg)	8.50e+06
Industrial Soil (mg/kg)	3.60e+07
Resident Air (ug/m3)	6.30e+00
Industrial Air (ug/m3)	2.60e+01
Chronic Inhalation Reference Concentration (mg/m3)	6.00e-03
Volatile	Volatile
Mutagen	Mutagen

Fraction of Contaminant Absorbed in Gastrointestinal Tract	1
Fraction of Contaminant Absorbed Dermally from Soil	0.1

EPA Regional Screening Levels for Chemical Contaminants at Superfund Sites

12.2.3 US EPA Regional Removal Management Levels for Chemical Contaminants

Resident Soil (mg/kg)	2.60e+07
Industrial Soil (mg/kg)	1.10e+08
Resident Air (ug/m3)	1.90e+01
Industrial Air (ug/m3)	7.90e+01
Chronic Inhalation Reference Concentration (mg/m3)	6.00e-03
Volatile	Volatile
Mutagen	Mutagen
Fraction of Contaminant Absorbed in Gastrointestinal Tract	1
Fraction of Contaminant Absorbed Dermally from Soil	0.1

EPA Regional Screening Levels for Chemical Contaminants at Superfund Sites

12.2.4 Environmental Fate / Exposure Summary

Adiponitrile's production and use as an intermediate in the manufacture of nylon, organic synthesis, and as an extractant for aromatic hydrocarbons may result in its release to the environment through various waste streams. If released to air, a vapor pressure of 6.79X10-4 mm Hg at 25 °C indicates adiponitrile will exist solely as a vapor in the ambient atmosphere. Vapor-phase adiponitrile will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to

be 23 days. If released to soil, adiponitrile is expected to have very high mobility based upon an estimated Koc of 16. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 1.21X10-9 atm-cu m/mole. Microorganisms isolated from soil were able to use adiponitrile as their sole source of carbon. If released into water, adiponitrile is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. Adiponitrile had a 5-day theoretical BOD of 40% in a river die-away study using unacclimated river water with a sewage inocula; the 12-day theoretical BOD was >100%. Thus, adiponitrile is expected to biodegrade in aquatic systems. Volatilization from water surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. An estimated BCF of 3 suggests the potential for bioconcentration in aquatic organisms is low. Chemical hydrolysis of adiponitrile is expected to be slow based on a chemical hydrolysis half-life of >150,000 yrs for acetonitrile. Occupational exposure to adiponitrile may occur by dermal contact with this compound at workplaces where adiponitrile is produced or used. (SRC)

- Hazardous Substances Data Bank (HSDB)

12.2.5 Artificial Pollution Sources

Adiponitrile's production and use as an intermediate in the manufacture of nylon(1), organic synthesis(1), and as an extractant for aromatic hydrocarbons(2) may result in its release to the environment through various waste streams(SRC).

(1) Lewis RJ Sr, ed; Hawley's Condensed Chemical Dictionary 13th ed. NY, NY: John Wiley and Sons Inc, p. 23 (1997)

(2) McKinney RJ, DeVito SC; Kirk-Othmer Encycl Chem Tech 4th ed. NY, NY: John Wiley and Sons, Supp: 447 (1998)

- Hazardous Substances Data Bank (HSDB)

12.2.6 Environmental Fate

TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 16(SRC), determined from a log Kow of -0.32(2) and a regression-derived equation(3), indicates that adiponitrile is expected to have very high mobility in soil(SRC). Volatilization of adiponitrile from moist soil surfaces is not expected to be an important fate process(SRC) given an estimated Henry's Law constant of 1.21X10-9 atm-cu m/mole(SRC), derived from its vapor pressure, 6.79X10-4 mm Hg(4), and water solubility, 8.00X10+4 mg/l(5). Adiponitrile is not expected to volatilize from dry soil surfaces(SRC) based upon its vapor pressure(4). In water, adiponitrile had a 5-day theoretical BOD of 40% in a river die-away study using unacclimated Ohio River water, 0.5-10 mg/l substrate concn and sewage inocula(6); the 12-day theoretical

BOD was >100%(6); negligible degradation was observed after 2 days(6). In addition, microorganisms (Aeromonas sp.) isolated from soil were able to use adiponitrile as its sole source of **carbon**(7). Thus, adiponitrile may be expected to biodegrade in soil systems(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983)

(2) Tanii H, Hashimoto K; Arch Toxicol 57: 88-93 (1985)

(3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9 (1990)

(4) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation. Design Inst Phys Prop Data, Amer Inst Chem Eng NY, NY: Hemisphere Pub Corp 5 Vol (1989)

(5) McKinney RJ, DeVito SC; Kirk-Othmer Encycl Chem Tech 4th ed. NY, NY: John Wiley and Sons, Supp: 444 (1998)

(6) Ludzack FJ et al; Sewage Ind Wastes 31: 33-44 (1959)

(7) Kuwahara M et al; Hakkokogaku Kaishi 58: 441-8 (1980)

Hazardous Substances Data Bank (HSDB)

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 16(SRC), determined from a log Kow of -0.32(2) and a regression-derived equation(3), indicates that adiponitrile is not expected to adsorb to suspended solids and sediment(SRC). Volatilization from **water** surfaces is not expected(3) based upon an estimated Henry's Law constant of 1.21X10-9 atm-cu m/mole(SRC), derived from its vapor pressure, 6.79X10-4 mm Hg(4), and **water** solubility, 8.00X10+4 mg/l(5). According to a classification scheme(6), an estimated BCF of 3(SRC), from its log Kow(2) and a regression-derived equation(7), suggests the potential for bioconcentration in aquatic organisms is low(SRC). Adiponitrile had a 5-day theoretical BOD of 40% in a river die-away study using unacclimated Ohio River **water**, 0.5-10 mg/l substrate concn and sewage inocula(8); the 12-day theoretical BOD was >100%(8); negligible degradation was observed after 2 days(8). Thus, adiponitrile is expected to biodegrade in aquatic systems(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983)

(2) Tanii H, Hashimoto K; Arch Toxicol 57: 88-93 (1985)

(3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9, 15-1 to 15-29 (1990)

(4) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation. Design Inst Phys Prop Data, Amer Inst Chem Eng NY, NY: Hemisphere Pub Corp 5 Vol (1989)

(5) McKinney RJ, DeVito SC; Kirk-Othmer Encycl Chem Tech 4th ed. NY, NY: John Wiley and Sons, Supp: 444 (1998)

(6) Franke C et al; Chemosphere 29: 1501-14 (1994)

(7) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999)

(8) Ludzack FJ et al; Sewage Ind Wastes 31: 33-44 (1959)

▸ Hazardous Substances Data Bank (HSDB)

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), adiponitrile, which has a vapor pressure of 6.79X10-4 mm Hg at 25 °C(2), is expected to exist solely as a vapor in the ambient atmosphere(SRC). Vapor-phase adiponitrile is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals(SRC); the half-life for this reaction in air is estimated to be 23 days(SRC), calculated from its rate constant of 7.12X10-13 cu cm/molecule-sec at 25 °C(SRC) determined using a structure estimation method(3).

(1) Bidleman TF; Environ Sci Technol 22: 361-367 (1988)

(2) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation. Design Inst Phys Prop Data, Amer Inst Chem Eng NY, NY: Hemisphere Pub Corp 5 Vol (1989)

(3) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993)

▸ Hazardous Substances Data Bank (HSDB)

12.2.7 Environmental Biodegradation

AEROBIC: Adiponitrile had a 5-day theoretical BOD of 40% in a river die-away study using unacclimated Ohio River **water**, 0.5-10 mg/l substrate concn and sewage inocula(1); a 12-day theoretical BOD was >100%(1); negligible degradation was observed after 2 days(1). At a substrate concn of 40 mg/l and 20 °C, adiponitrile had theoretical CO2 evolutions of 10 and 60% after 2 and 9 days, respectively, in river die-away studies using unacclimated Ohio River **water** and sewage inocula(1); at 5 °C, theoretical CO2 evolution was 10 and 60% after 7.5 and 33 days, respectively(1). At 20 °C, effects of acclimation were examined by redosing at an initial substrate concn of 40 mg/l; the ratio of time it took to achieve 60% oxidation on 1st and 2nd feeding was 2.1 to 1(1). Adiponitrile was found to be toxic to one activated sludge unit after 72 hrs with a metal substrate concn of 500 mg/l; the other two sludge units had 2.2-2.8% theoretical BOD(2). Using a bench scale activated sludge unit, 93-98% BOD removal of adiponitrile was achieved using an influent concn equivalent to 275-350 mg/l BOD and a mean aeration retention time of 7-13 hours(3). Adiponitrile, present at 30 mg/l, reached 85% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 100 mg/l and the Japanese MITI test(4). Microorganisms (Aeromonas sp.) isolated from soil were able to use adiponitrile as their sole source of **carbon**(5).

(1) Ludzack FJ et al; Sewage Ind Wastes 31: 33-44 (1959)

(2) Lutin PA; J Water Poll Contr Fed 42: 1632-42 (1970)

(3) Ludzack FJ et al; Proc of the 14th Industrial Waste Conf, Eng Ext Ser 104: 547-65 (1959)

*(4) CITI; Biodegradation and Bioaccumulation Data of Existing Chemicals Database on Adiponitrile (111-69-3). Available from the Database Query page at **https://www.cerij.or.jp/ceri_en/index_e4.shtml** as of Jan 1,*

2001.

(5) Kuwahara M et al; Hakkokogaku Kaishi 58: 441-8 (1980)

- **Hazardous Substances Data Bank (HSDB)**

12.2.8 Environmental Abiotic Degradation

The rate constant for the vapor-phase reaction of adiponitrile with photochemically-produced hydroxyl radicals has been estimated as 7.12X10-13 cu cm/molecule-sec at 25 °C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 23 days at an atmospheric concentration of 5X10+5 hydroxyl radicals per cu cm(1). Chemical hydrolysis is expected to be slow, based on a chemical hydrolysis half-life of >150,000 yrs for **acetonitrile**(2). Adiponitrile is not expected to directly photolyze due to the lack of absorption in the environmental UV spectrum (>290 nm)(SRC).

(1) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993)

(2) Ellington JJ et al; Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal. Vol 3 USEPA/600/3-88/028 p. 18 (1988)

- **Hazardous Substances Data Bank (HSDB)**

12.2.9 Environmental Bioconcentration

An estimated BCF of 3 was calculated for adiponitrile(SRC), using a log Kow of -0.32(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

(1) Tanii H, Hashimoto K; Arch Toxicol 57: 88-93 (1985)

(2) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999)

(3) Franke C et al; Chemosphere 29: 1501-14 (1994)

- **Hazardous Substances Data Bank (HSDB)**

12.2.10 Soil Adsorption / Mobility

The Koc of adiponitrile is estimated as 16(SRC), using a measured log Kow of -0.32(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that adiponitrile is expected to have very high mobility in soil(SRC).

(1) Tanii H, Hashimoto K; Arch Toxicol 57: 88-93 (1985)

(2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9 (1990)

(3) Swann RL et al; Res Rev 85: 17-28 (1983)

- Hazardous Substances Data Bank (HSDB)

12.2.11 Volatilization from Water / Soil

The Henry's Law constant for adiponitrile is estimated as 1.21X10-9 atm-cu m/mole(SRC) derived from its vapor pressure, 6.79X10-4 mm Hg(1), and water solubility, 8.00X10+4 mg/l(2). This Henry's Law constant indicates that adiponitrile is expected to be essentially nonvolatile from moist soil and water surfaces(3). Adiponitrile is not expected to volatilize from dry soil surfaces(SRC) based upon its vapor pressure(1).

(1) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation. Design Inst Phys Prop Data, Amer Inst Chem Eng NY, NY: Hemisphere Pub Corp 5 Vol (1989)

(2) McKinney RJ, DeVito SC; Kirk-Othmer Encycl Chem Tech 4th ed. NY, NY: John Wiley and Sons, Supp: 444 (1998)

(3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990)

- Hazardous Substances Data Bank (HSDB)

12.2.12 Environmental Water Concentrations

DRINKING WATER: Adiponitrile was tentatively identified in drinking water collected in New Orleans, LA on Jan 14, 1976(1).

(1) Lucas SV; GC/MS Analysis of Organics in Drinking Water Concentrates and Advanced Waste Treatment Concentrates: Vol 2. Computer-Printed Tabulations of Compound Identification Results for Large-Volume Concentrates USEPA-600/1-84- 020B NTIS PB-128239 p.10 (1984)

- Hazardous Substances Data Bank (HSDB)

12.2.13 Effluent Concentrations

Identified in effluent from a nylon manufacturing plant during Aug 1973(1).

(1) Shackelford WM, Keith LH; Frequency of Organic Compounds Identified in Water USEPA-600/4-76-062 p. 56 (1976)

- Hazardous Substances Data Bank (HSDB)

12.2.14 Probable Routes of Human Exposure

NIOSH (NOES Survey 1981-1983) has statistically estimated that 478 workers (41 of these are female) are potentially exposed to adiponitrile in the US(1). Occupational exposure to adiponitrile may occur by dermal contact(2) with this compound at workplaces where adiponitrile is produced or used(SRC).

(1) NIOSH; National Occupational Exposure Survey (NOES) (1983)

(2) Parmeggiani L, ed; Encycl of Occup Health and Safety 3rd ed Geneva, Switzerland: Intern Labour Organ 2: 1446-7 (1983)

- **Hazardous Substances Data Bank (HSDB)**

13 Literature

13.1 Consolidated References

- **PubChem**

13.2 NLM Curated PubMed Citations

PubChem

13.3 Springer Nature References

Springer Nature

13.4 Thieme References

Thieme Chemistry

13.5 Chemical Co-Occurrences in Literature

PubChem

13.6 Chemical-Gene Co-Occurrences in Literature

PubChem

13.7 Chemical-Disease Co-Occurrences in Literature

PubChem

14 Patents

14.1 Depositor-Supplied Patent Identifiers

- PubChem

Link to all deposited patent identifiers

- PubChem

14.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=BTGRAWJCKBQKAO-UHFFFAOYSA-N

- PATENTSCOPE (WIPO)

14.3 Chemical Co-Occurrences in Patents

- PubChem

14.4 Chemical-Disease Co-Occurrences in Patents

PubChem

14.5 Chemical-Gene Co-Occurrences in Patents

PubChem

15 Interactions and Pathways

15.1 Chemical-Target Interactions

- Toxin and Toxin Target Database (T3DB)

16 Biological Test Results

16.1 BioAssay Results

- PubChem

17 Classification

17.1 MeSH Tree

- Medical Subject Headings (MeSH)

17.2 ChemIDplus

- ChemIDplus

17.3 CAMEO Chemicals

- CAMEO Chemicals

17.4 UN GHS Classification

- GHS Classification (UNECE)

17.5 NORMAN Suspect List Exchange Classification

- NORMAN Suspect List Exchange

17.6 EPA DSSTox Classification

- EPA DSSTox

17.7 EPA TSCA and CDR Classification

- EPA Chemicals under the TSCA

17.8 EPA Substance Registry Services Tree

EPA Substance Registry Services

17.9 MolGenie Organic Chemistry Ontology

MolGenie

18 Information Sources

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1. ## Australian Industrial Chemicals Introduction Scheme (AICIS)

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Hexanedinitrile

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CAMEO Chemical Reactivity Classification

https://cameochemicals.noaa.gov/browse/react

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https://www.ilo.org/dyn/icsc/showcard.display?p_version=2&p_card_id=0211

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Adiponitrile

https://commonchemistry.cas.org/detail?cas_rn=111-69-3

5. ## ChemIDplus

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Adiponitrile

https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0000111693

Hexanedinitrile, hydrogenated, high-boiling fraction

https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0068411905

ChemIDplus Chemical Information Classification

https://pubchem.ncbi.nlm.nih.gov/source/ChemIDplus

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Hexanedinitrile

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https://www.epa.gov/chemicals-under-tsca

EPA TSCA Classification

https://www.epa.gov/tsca-inventory

9. ## EPA DSSTox

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https://comptox.epa.gov/dashboard/DTXSID3021936

CompTox Chemicals Dashboard Chemical Lists

https://comptox.epa.gov/dashboard/chemical-lists/

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https://iris.epa.gov/ChemicalLanding/&substance_nmbr=515

11. ## EPA Provisional Peer-Reviewed Toxicity Values (PPRTVs)

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Adiponitrile

https://cfpub.epa.gov/ncea/pprtv/chemicalLanding.cfm?pprtv_sub_id=1557

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https://chem.echa.europa.eu/100.003.543

Adiponitrile (EC: 203-896-3)

https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/51231

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https://gsrs.ncats.nih.gov/ginas/app/beta/substances/SYT33B891I

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https://pubchem.ncbi.nlm.nih.gov/source/hsdb/627

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https://www.epa.govt.nz/industry-areas/hazardous-substances/guidance-for-importers-and-manufacturers/hazardous-substances-databases/

16. NJDOH RTK Hazardous Substance List

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http://nj.gov/health/eoh/rtkweb/documents/fs/0027.pdf

17. Occupational Safety and Health Administration (OSHA)

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https://www.osha.gov/chemicaldata/129

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https://rais.ornl.gov/cgi-bin/tools/TOX_search

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https://www.cdc.gov/niosh/npg/npgd0015.html

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https://haz-map.com/About

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https://haz-map.com/Agents/160

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http://www.t3db.ca/toxins/T3D1689

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http://www.ebi.ac.uk/Information/termsofuse.html

https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL2132938/

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https://www.crystallography.net/cod/2020899.html

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https://epa-prgs.ornl.gov/cgi-bin/chemicals/csl_search

Adiponitrile

https://epa-prgs.ornl.gov/cgi-bin/chemicals/csl_search?tool=rml

26. NITE-CMC

Adiponitrile - FY2009 (Revised classification)

https://www.nite.go.jp/chem/english/ghs/09-mhlw-2059e.html

Adiponitrile - FY2006 (New/original classication)

https://www.nite.go.jp/chem/english/ghs/06-imcg-0005e.html

27. NMRShiftDB

https://pubchem.ncbi.nlm.nih.gov/substance/589867

28. MassBank Europe

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https://github.com/MassBank/MassBank-web/blob/main/MassBank-Project/LICENSE.txt

1,4-BUTANEDICARBONITRILE

https://massbank.eu/MassBank/Result.jsp?inchikey=BTGRAWJCKBQKAO-UHFFFAOYSA-N

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Adiponitrile

http://www.hmdb.ca/metabolites/HMDB0248015

HMDB0248015_nmr_one_2155

https://hmdb.ca/metabolites/HMDB0248015#spectra

30. SpectraBase

ADIPONITRILE

https://spectrabase.com/spectrum/6nyDBtrMBlD

adiponitrile

https://spectrabase.com/spectrum/B5G5rMpdBGl

ADIPONITRILE

https://spectrabase.com/spectrum/4GbfEJkOIno

ADIPONITRILE

https://spectrabase.com/spectrum/7pB3XVsoyMa

HEXANEDINITRILE

https://spectrabase.com/spectrum/Z4HI7vAxhN

HEXANEDINITRILE

https://spectrabase.com/spectrum/3dFDY7roRUC

ADIPONITRILE

https://spectrabase.com/spectrum/FRSm5b0IRyF

1,4-Dicyanobutane

https://spectrabase.com/spectrum/Gg8x1Y7zhDH

ADIPONITRILE

https://spectrabase.com/spectrum/JrOvGN25pfW

ADIPONITRILE

https://spectrabase.com/spectrum/Fx7L215vdHv

Adiponitrile

https://spectrabase.com/spectrum/J75L6AakPuJ

Adiponitrile

https://spectrabase.com/spectrum/1ApLcMFryff

31. Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J2.456B

32. MassBank of North America (MoNA)

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1,4-BUTANEDICARBONITRILE

https://mona.fiehnlab.ucdavis.edu/spectra/browse?

query=exists(compound.metaData.name:%27InChIKey%27%20and%20compound.metaData.value:%27BTGRAWJCKBQKAO-UHFFFAOYSA-N%27)

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Hexanedinitrile

http://www.nist.gov/srd/nist1a.cfm

34. Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=8041128-239380860

35. SpringerMaterials

hexanedinitrile

https://materials.springer.com/substanceprofile/docs/smsid_bohrfgfycqwosrfu

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adiponitrile

https://www.wikidata.org/wiki/Q84062

38. ## Wikipedia

Adiponitrile

https://en.wikipedia.org/wiki/Adiponitrile

39. PubChem

https://pubchem.ncbi.nlm.nih.gov

40. ## Medical Subject Headings (MeSH)

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adiponitrile

https://www.ncbi.nlm.nih.gov/mesh/67036546

MeSH Tree

http://www.nlm.nih.gov/mesh/meshhome.html

41. ## GHS Classification (UNECE)

GHS Classification Tree

http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

42. ## NORMAN Suspect List Exchange

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NORMAN Suspect List Exchange Classification

https://www.norman-network.com/nds/SLE/

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EPA SRS List Classification

https://sor.epa.gov/sor_internet/registry/substreg/LandingPage.do

44. ## MolGenie

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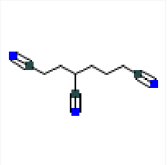
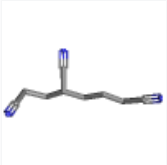
MolGenie Organic Chemistry Ontology
https://github.com/MolGenie/ontology/

45. PATENTSCOPE (WIPO)

SID 403031314
https://pubchem.ncbi.nlm.nih.gov/substance/403031314

COMPOUND SUMMARY

1,3,6-Tricyanohexane

PubChem CID	15678
Structure	 2D  3D
Chemical Safety	Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_9H_{11}N_3$
Synonyms	1,3,6-Hexanetricarbonitrile 1772-25-4 hexane-1,3,6-tricarbonitrile 1,3,6-TRICYANOHEXANE 4-Cyanosuberonitrile View More...
Molecular Weight	161.20 g/mol *Computed by PubChem 2.2 (PubChem release 2021.10.14)*
Dates	Create: 2005-08-08 Modify: 2024-10-26

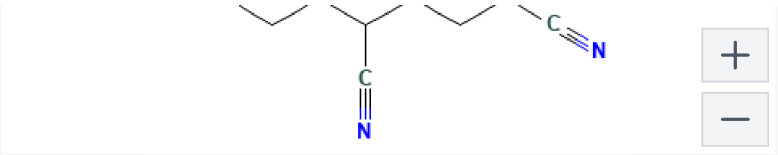
Contents

Title and Summary
1 Structures
2 Names and Identifiers
3 Chemical and Physical Properties
4 Spectral Information
5 Related Records
6 Chemical Vendors
7 Use and Manufacturing
8 Safety and Hazards
9 Toxicity
10 Literature
11 Patents
12 Biological Test Results
13 Classification
14 Information Sources

1 Structures

1.1 2D Structure

Chemical Structure Depiction



PubChem

1.2 3D Conformer

PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

hexane-1,3,6-tricarbonitrile

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PubChem

2.1.2 InChI

InChI=1S/C9H11N3/c10-6-2-1-4-9(8-12)5-3-7-11/h9H,1-5H2

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

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2.1.3 InChIKey

LNLFLMCWDHZINJ-UHFFFAOYSA-N

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2.1.4 SMILES

C(CC#N)CC(CCC#N)C#N

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PubChem

2.2 Molecular Formula

$C_9H_{11}N_3$

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2.3 Other Identifiers

2.3.1 CAS

1772-25-4

CAS Common Chemistry; ChemIDplus; EPA Chemical Data Reporting (CDR); EPA Chemicals under…

2.3.2 European Community (EC) Number

217-199-7

- European Chemicals Agency (ECHA)

2.3.3 UNII

SJY3YNQ3SI

- FDA Global Substance Registration System (GSRS)

2.3.4 ChEMBL ID

CHEMBL3183751

- ChEMBL

2.3.5 DSSTox Substance ID

DTXSID4041234

- EPA DSSTox

2.3.6 Nikkaji Number

J27.810F

- Japan Chemical Substance Dictionary (Nikkaji)

2.3.7 Wikidata

Q27289244

- Wikidata

2.4 Synonyms

2.4.1 Depositor-Supplied Synonyms

1,3,6-Hexanetricarbonitrile	DTXCID2021234	AKOS022182701
1772-25-4	1,3,6-TRICYANOHEXANE [HSDB]	s12371

hexane-1,3,6-tricarbonitrile	4cyanosuberonitrile	NCGC00248239-01
1,3,6-TRICYANOHEXANE	MFCD00129792	NCGC00254878-01
4-Cyanosuberonitrile	(+/-)-1,3,6-HEXANETRICARBONITRILE, TECH. , 80+%	BS-21827
SJY3YNQ3SI	1,3,6Hexanetricarbonitrile	CAS-1772-25-4
UNII-SJY3YNQ3SI	SCHEMBL1323168	CS-0198995
HSDB 5855	CHEMBL3183751	H1504
DTXSID4041234	BAA77225	NS00025841
EINECS 217-199-7	Tox21_300976	Q27289244

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	161.20 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
XLogP3-AA	0.4	Computed by XLogP3 3.0 (PubChem release 2021.10.14)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Hydrogen Bond Acceptor Count	3	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Rotatable Bond Count	5	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Exact Mass	161.095297364 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Monoisotopic Mass	161.095297364 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Topological Polar Surface Area	71.4Å^2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Heavy Atom Count	12	Computed by PubChem
Formal Charge	0	Computed by PubChem

Complexity	253	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	1	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.10.14)

PubChem

3.2 Experimental Properties

3.2.1 Physical Description

Liquid; [MSDSonline]

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

3.3 Chemical Classes

Nitrogen Compounds -> Nitriles

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

4 Spectral Information

4.1 1D NMR Spectra

4.1.1 1H NMR Spectra

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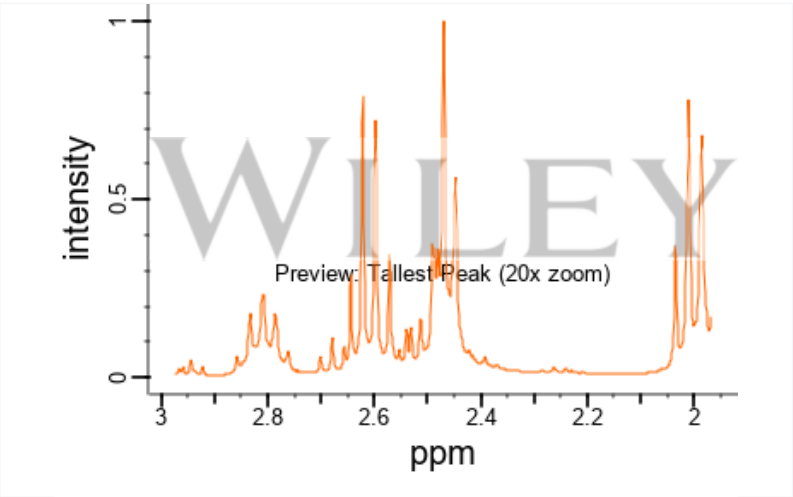
Thumbnail	

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4.1.2 13C NMR Spectra

1 of 2	
Instrument Name	Bruker AM-270
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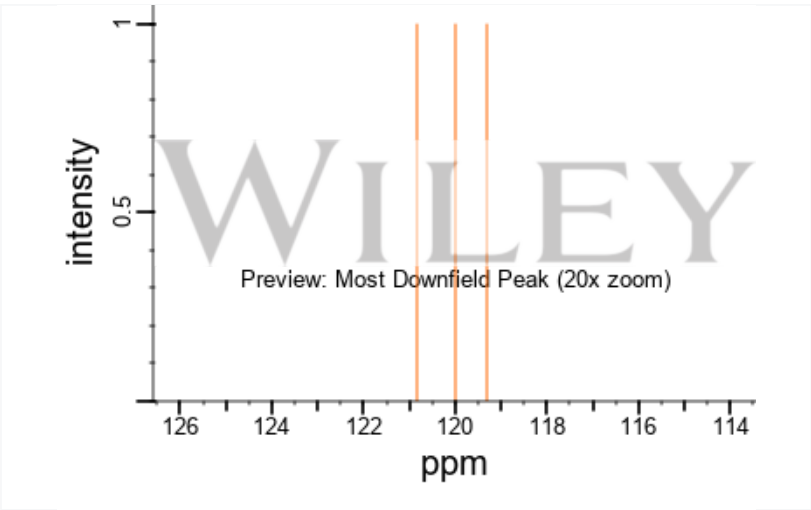
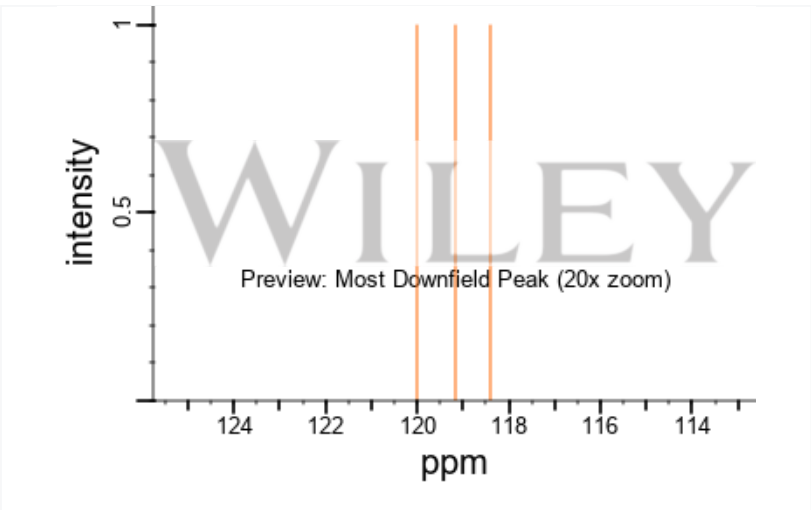
Thumbnail	

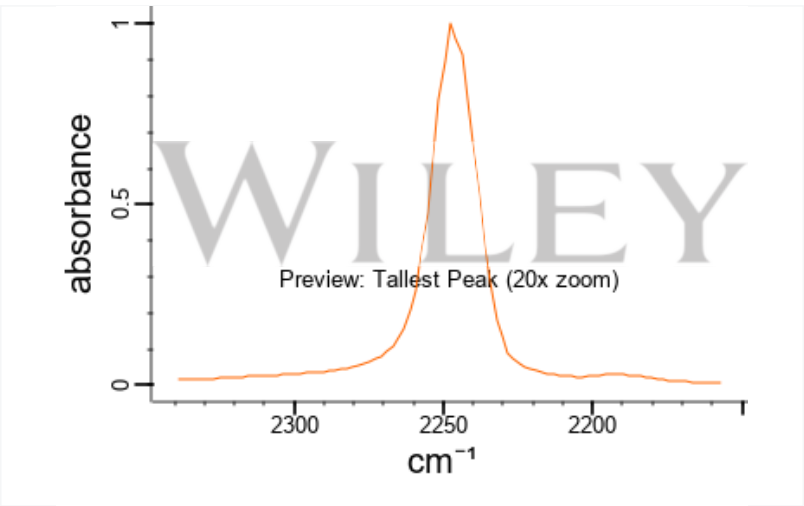
SpectraBase

2 of 2	
Instrument Name	Bruker AM-270
Copyright	Copyright © 2002-2024 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
Thumbnail	

SpectraBase

4.2 IR Spectra

4.2.1 FTIR Spectra

Instrument Name	Bruker IFS 85
Technique	Film
Copyright	Copyright © 1989, 1990-2024 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
Thumbnail	

- SpectraBase

5 Related Records

5.1 Related Compounds with Annotation

Follow these links to do a live 2D search or do a live 3D search for this compound, sorted by annotation score. This section is deprecated (see here for details), but these live search links provide equivalent functionality to the table that was previously shown here.

- PubChem

5.2 Related Compounds

Same Connectivity Count	3

Same Parent, Connectivity Count	3
Similar Compounds (2D)	View in PubChem Search
Similar Conformers (3D)	View in PubChem Search

PubChem

5.3 Substances

5.3.1 PubChem Reference Collection SID

500715813

PubChem

5.3.2 Related Substances

Same Count	91

PubChem

5.3.3 Substances by Category

PubChem

6 Chemical Vendors

PubChem

7 Use and Manufacturing

7.1 Uses

Sources/Uses

Not commercially used or produced in the US; [HSDB]

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

NO EVIDENCE OF COMMERCIAL USE IN U.S.

SRI

Hazardous Substances Data Bank (HSDB)

7.1.1 Industry Uses

Other

Stabilizing agent

https://www.epa.gov/chemical-data-reporting

- EPA Chemical Data Reporting (CDR)

7.2 Methods of Manufacturing

REACTION OF 1,3,6-TRICHLOROHEXANE WITH SODIUM CYANIDE (LABORATORY SYNTHESIS)

SRI

- Hazardous Substances Data Bank (HSDB)

7.3 U.S. Production

Aggregated Product Volume

2019: <1,000,000 lb

2018: <1,000,000 lb

2017: <1,000,000 lb

2016: <1,000,000 lb

https://www.epa.gov/chemical-data-reporting

- EPA Chemical Data Reporting (CDR)

(1979) NOT PRODUCED COMMERCIALLY IN U.S.

SRI

- Hazardous Substances Data Bank (HSDB)

(1981) NOT PRODUCED COMMERCIALLY IN U.S.

SRI

- Hazardous Substances Data Bank (HSDB)

7.4 U.S. Imports

(1979) No Data

SRI

- Hazardous Substances Data Bank (HSDB)

(1981) No Data

SRI

- Hazardous Substances Data Bank (HSDB)

7.5 U.S. Exports

(1979) No Data

SRI

- Hazardous Substances Data Bank (HSDB)

(1981) No Data

SRI

- Hazardous Substances Data Bank (HSDB)

7.6 General Manufacturing Information

Industry Processing Sectors

All Other Basic Organic Chemical Manufacturing
Other (requires additional information)

- EPA Chemical Data Reporting (CDR)

EPA TSCA Commercial Activity Status

1,3,6-Hexanetricarbonitrile: ACTIVE

- EPA Chemicals under the TSCA

8 Safety and Hazards

8.1 Hazards Identification

8.1.1 GHS Classification

Pictogram(s)	 Irritant
Signal	Warning
GHS Hazard Statements	H302 (97.6%): Harmful if swallowed [**Warning** Acute toxicity, oral] H332 (92.9%): Harmful if inhaled [**Warning** Acute toxicity, inhalation]
Precautionary Statement Codes	P261, P264, P270, P271, P301+P317, P304+P340, P317, P330, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided per 42 reports by companies from 3 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

- European Chemicals Agency (ECHA)

8.1.2 Hazard Classes and Categories

Acute Tox. 4 (97.6%)

Acute Tox. 4 (92.9%)

- European Chemicals Agency (ECHA)

8.1.3 Hazards Summary

May cause irritation; Targets kidneys and nerves; Harmful by ingestion and inhalation; [Aldrich MSDS] See NITRILES.

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

8.2 Regulatory Information

REACH Registered Substance

Status: Active Update: 22-02-2023 https://echa.europa.eu/registration-dossier/-/registered-dossier/33362

- European Chemicals Agency (ECHA)

9 Toxicity

9.1 Toxicological Information

9.1.1 Adverse Effects

Other Poison - Chemical Asphyxiant

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

10 Literature

10.1 Consolidated References

- PubChem

10.2 Springer Nature References

Springer Nature

10.3 Chemical Co-Occurrences in Literature

PubChem

11 Patents

11.1 Depositor-Supplied Patent Identifiers

PubChem

Link to all deposited patent identifiers

PubChem

11.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=LNLFLMCWDHZINJ-UHFFFAOYSA-N

PATENTSCOPE (WIPO)

11.3 Chemical Co-Occurrences in Patents

PubChem

11.4 Chemical-Disease Co-Occurrences in Patents

PubChem

11.5 Chemical-Gene Co-Occurrences in Patents

PubChem

12 Biological Test Results

12.1 BioAssay Results

PubChem

13 Classification

13.1 ChemIDplus

ChemIDplus

13.2 UN GHS Classification

GHS Classification (UNECE)

13.3 NORMAN Suspect List Exchange Classification

NORMAN Suspect List Exchange

13.4 EPA DSSTox Classification

EPA DSSTox

13.5 EPA TSCA and CDR Classification

EPA Chemicals under the TSCA

13.6 EPA Substance Registry Services Tree

EPA Substance Registry Services

14 Information Sources

FILTER BY SOURCE

ALL SOURCES

1. **CAS Common Chemistry**

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1,3,6-Hexanetricarbonitrile
https://commonchemistry.cas.org/detail?cas_rn=1772-25-4

2. **ChemIDplus**

LICENSE
https://www.nlm.nih.gov/copyright.html

1,3,6-Tricyanohexane
https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0001772254

ChemIDplus Chemical Information Classification
https://pubchem.ncbi.nlm.nih.gov/source/ChemIDplus

3. **EPA Chemical Data Reporting (CDR)**

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1,3,6-Hexanetricarbonitrile

https://www.epa.gov/chemical-data-reporting

4. EPA Chemicals under the TSCA

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

1,3,6-Hexanetricarbonitrile

https://www.epa.gov/chemicals-under-tsca

EPA TSCA Classification

https://www.epa.gov/tsca-inventory

5. EPA DSSTox

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

1,3,6-Hexanetricarbonitrile

https://comptox.epa.gov/dashboard/DTXSID4041234

CompTox Chemicals Dashboard Chemical Lists

https://comptox.epa.gov/dashboard/chemical-lists/

6. European Chemicals Agency (ECHA)

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https://echa.europa.eu/web/guest/legal-notice

Hexane-1,3,6-tricarbonitrile

https://chem.echa.europa.eu/100.015.636

Hexane-1,3,6-tricarbonitrile (EC: 217-199-7)

https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/117080

7. FDA Global Substance Registration System (GSRS)

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https://www.fda.gov/about-fda/about-website/website-policies#linking

1,3,6-TRICYANOHEXANE

https://gsrs.ncats.nih.gov/ginas/app/beta/substances/SJY3YNQ3SI

8. ## Hazardous Substances Data Bank (HSDB)

LICENSE
https://www.nlm.nih.gov/web_policies.html

1,3,6-TRICYANOHEXANE

https://pubchem.ncbi.nlm.nih.gov/source/hsdb/5855

9. ## ChEMBL

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http://www.ebi.ac.uk/Information/termsofuse.html

https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL3183751/

10. ## Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

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https://haz-map.com/About

1,3,6-Tricyanohexane

https://haz-map.com/Agents/2780

11. ## Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J27.810F

12. ## SpectraBase

1,3,6-Tricyano-hexane

https://spectrabase.com/spectrum/D5DibHjs8DY

1,3,6-Tricyano-hexane

https://spectrabase.com/spectrum/GGNVsCDynjp

1,3,6-Hexanetricarbonitrile

https://spectrabase.com/spectrum/C5dTZbmXzhG

1,3,6-Hexanetricarbonitrile

https://spectrabase.com/spectrum/66YPZR3QEFZ

13. ## Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=12051232-209212740

14. ## Wikidata

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CCZero
https://creativecommons.org/publicdomain/zero/1.0/

1,3,6-tricyanohexane
https://www.wikidata.org/wiki/Q27289244

15. PubChem

https://pubchem.ncbi.nlm.nih.gov

16. GHS Classification (UNECE)

GHS Classification Tree
http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

17. NORMAN Suspect List Exchange

LICENSE
Data: CC-BY 4.0; Code (hosted by ECI, LCSB): Artistic-2.0
https://creativecommons.org/licenses/by/4.0/

NORMAN Suspect List Exchange Classification
https://www.norman-network.com/nds/SLE/

18. EPA Substance Registry Services

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

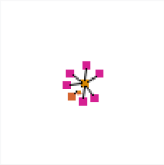
EPA SRS List Classification
https://sor.epa.gov/sor_internet/registry/substreg/LandingPage.do

19. PATENTSCOPE (WIPO)

SID 388341353
https://pubchem.ncbi.nlm.nih.gov/substance/388341353

COMPOUND SUMMARY

Lithium hexafluorophosphate

PubChem CID	23688915
Structure	 2D
Chemical Safety	Corrosive, Acute Toxic, Irritant, Health Hazard Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$F_6P.Li$ F_6LiP
Synonyms	Lithium hexafluorophosphate 21324-40-3 Lithium hexafluorophosphate(V) LiPF6 lithium,hexafluorophosphate View More...
Molecular Weight	151.9 g/mol *Computed by PubChem 2.2 (PubChem release 2021.10.14)*
Component Compounds	CID 9886 (Hexafluorophosphate) CID 3028194 (Lithium)

Dates	Create: 2008-02-05	Modify: 2024-10-26
Description	Lithium hexafluorophosphate is an inorganic lithium salt having hexafluorophosphate(1-) as the counterion. It is an electrolyte used in lithium-ion batteries. It contains a hexafluorophosphate(1-). ▸ ChEBI	

Contents

Title and Summary

1 Structures

2 Names and Identifiers

3 Chemical and Physical Properties

4 Spectral Information

5 Related Records

6 Chemical Vendors

7 Use and Manufacturing

8 Safety and Hazards

9 Toxicity

10 Literature

11 Patents

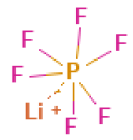
12 Classification

13 Information Sources

1 Structures

1.1 2D Structure

Chemical Structure Depiction



PubChem

1.2 3D Status

Conformer generation is disallowed since MMFF94s unsupported element, mixture or salt

PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

lithium;hexafluorophosphate

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

PubChem

2.1.2 InChI

InChI=1S/F6P.Li/c1-7(2,3,4,5)6;/q-1;+1

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

PubChem

2.1.3 InChIKey

AXPLOJNSKRXQPA-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

PubChem

2.1.4 SMILES

[Li+].F[P-](F)(F)(F)(F)F

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

PubChem

2.2 Molecular Formula

$F_6P.Li$

Australian Industrial Chemicals Introduction Scheme (AICIS)

F_6LiP

Computed by PubChem 2.2 (PubChem release 2021.10.14)

PubChem

2.3 Other Identifiers

2.3.1 CAS

21324-40-3

Australian Industrial Chemicals Introduction Scheme (AICIS); CAS Common Chemistry; ChemIDpl···

2.3.2 Deprecated CAS

195377-88-9, 2028300-39-0, 2511147-71-8, 285996-05-6, 499988-42-0, 672306-79-5, 79001-09-5

- ChemIDplus; EPA Chemicals under the TSCA

285996-05-6, 499988-42-0, 672306-79-5, 79001-09-5

- EPA DSSTox

2.3.3 European Community (EC) Number

244-334-7

- European Chemicals Agency (ECHA)

2.3.4 UNII

T9T8DY51J3

- FDA Global Substance Registration System (GSRS)

2.3.5 ChEBI ID

CHEBI:172376

- ChEBI

2.3.6 DSSTox Substance ID

DTXSID2066698

- EPA DSSTox

2.3.7 Wikidata

Q2583808

- Wikidata

2.3.8 Wikipedia

Lithium hexafluorophosphate

- Wikipedia

2.4 Synonyms

2.4.1 Depositor-Supplied Synonyms

Lithium hexafluorophosphate	Phosphate(1-), hexafluoro-, lithium (1:1)	Lithiumhexafluoroph
21324-40-3	CHEBI:172376	Lithium hexafluoroph
Lithium hexafluorophosphate(V)	EINECS 244-334-7	hexafluorophosphate
LiPF6	LBG-45864	DTXCID6036463
lithium,hexafluorophosphate	MFCD00011096	Lithium hexafluoroph
lithium;hexafluorophosphate	LITHIUM HEXAFLUOROPHOSPHATE [MI]	Phosphate(1), hexaflu
Phosphate(1-), hexafluoro-, lithium	LITHIUM HEXAFLUOROPHOSPHATE (LIPF6)	AKOS015833778
T9T8DY51J3	EC 244-334-7	GS-3314
UNII-T9T8DY51J3	Lithium hexafluorophosphate(1-)	Lithium hexafluoroph
DTXSID2066698	Lithium phosphohexafluoride	Lithium hexafluoroph

- PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	151.9 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Hydrogen Bond Acceptor Count	7	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Rotatable Bond Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Exact Mass	151.98018440 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Monoisotopic Mass	151.98018440 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Topological Polar Surface Area	0Å^2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Heavy Atom Count	8	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	67.1	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	2	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.10.14)

PubChem

3.2 Experimental Properties

3.2.1 Physical Description

Other Solid; Pellets or Large Crystals; Dry Powder

EPA Chemical Data Reporting (CDR)

White to almost white hygroscopic powder; [Acros Organics MSDS]

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

3.3 Chemical Classes

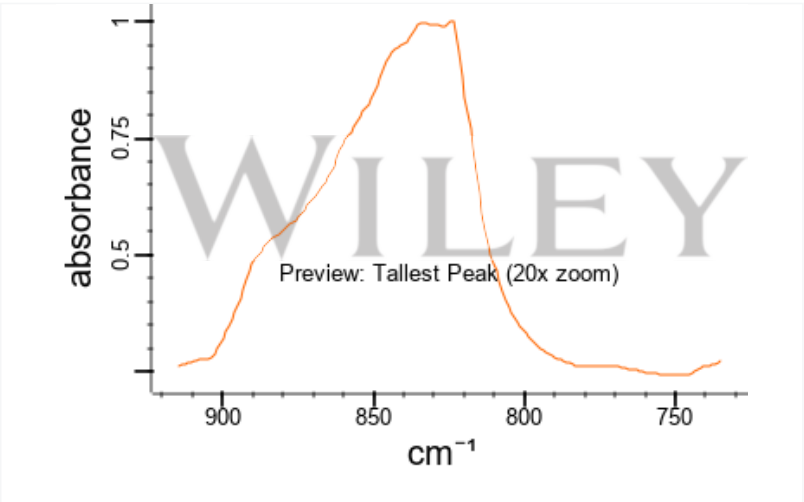
Metals -> Metals, Inorganic Compounds

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

4 Spectral Information

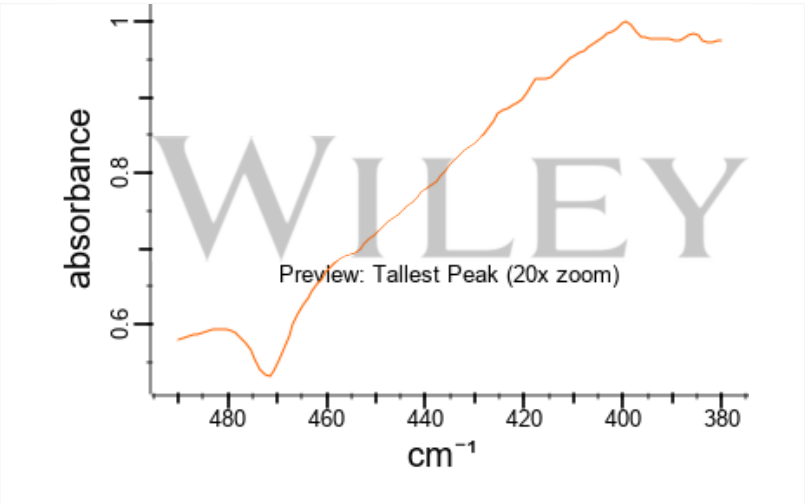
4.1 IR Spectra

4.1.1 FTIR Spectra

Technique	SPLIT MULL
Source of Sample	PCR, Inc., Gainesville, Florida
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

- SpectraBase

4.1.2 ATR-IR Spectra

Instrument Name	Bruker Tensor 27 FT-IR
Technique	ATR-Neat
Source of Spectrum	Bio-Rad Laboratories, Inc.
Source of Sample	Alfa Aesar, Thermo Fisher Scientific
Catalog Number	11529
Lot Number	Y30B038
Copyright	Copyright © 2018-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

- SpectraBase

5 Related Records

5.1 Related Compounds with Annotation

Follow these links to **do a live 2D search** or **do a live 3D search** for this compound, sorted by annotation score. This section is deprecated (see **here** for details), but these live search links provide equivalent functionality to the table that was previously shown here.

- PubChem

5.2 Component Compounds

CID 9886 (Hexafluorophosphate)

CID 3028194 (Lithium)

PubChem

5.3 Related Compounds

Same Connectivity Count	3
Mixtures, Components, and Neutralized Forms Count	2
Similar Compounds (2D)	View in PubChem Search
Similar Conformers (3D)	View in PubChem Search

PubChem

5.4 Substances

5.4.1 PubChem Reference Collection SID

500797140

PubChem

5.4.2 Related Substances

Same Count	129

PubChem

5.4.3 Substances by Category

PubChem

6 Chemical Vendors

PubChem

7 Use and Manufacturing

7.1 Uses

EPA CPDat Chemical and Product Categories

The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products, Scientific Data, volume 5, Article number: 180125 (2018), ***DOI:10.1038/sdata.2018.125***

- EPA Chemical and Products Database (CPDat)

7.1.1 Industry Uses

Conductive agent
Not Known or Reasonably Ascertainable
Solvents (which become part of product formulation or mixture)

https://www.epa.gov/chemical-data-reporting

- EPA Chemical Data Reporting (CDR)

7.1.2 Consumer Uses

Conductive agent

https://www.epa.gov/chemical-data-reporting

- EPA Chemical Data Reporting (CDR)

7.2 U.S. Production

Aggregated Product Volume

2019: 1,000,000 lb - <20,000,000 lb

2018: 1,000,000 lb - <20,000,000 lb

2017: 1,000,000 lb - <20,000,000 lb

2016: 100,000 - <500,000 lb

https://www.epa.gov/chemical-data-reporting

- EPA Chemical Data Reporting (CDR)

7.3 General Manufacturing Information

Industry Processing Sectors

All Other Chemical Product and Preparation Manufacturing
Not Known or Reasonably Ascertainable

- EPA Chemical Data Reporting (CDR)

EPA TSCA Commercial Activity Status

Phosphate(1-), hexafluoro-, lithium (1:1): ACTIVE

- EPA Chemicals under the TSCA

EPA TSCA Regulatory Flag

PMN - indicates a commenced PMN (Pre-Manufacture Notices) substance.

https://www.epa.gov/tsca-inventory

- EPA Chemicals under the TSCA

8 Safety and Hazards

8.1 Hazards Identification

8.1.1 GHS Classification

Pictogram(s)	Corrosive Acute Toxic Irritant Health Hazard
Signal	**Danger**
GHS Hazard Statements	H301 (81.3%): Toxic if swallowed [**Danger** Acute toxicity, oral] H302 (18.7%): Harmful if swallowed [**Warning** Acute toxicity, oral] H311 (15%): Toxic in contact with skin [**Danger** Acute toxicity, dermal] H314 (100%): Causes severe skin burns and eye damage [**Danger** Skin corrosion/irritation] H318 (72.3%): Causes serious eye damage [**Danger** Serious eye damage/eye irritation] H372 (69.5%): Causes damage to organs through prolonged or repeated exposure [**Danger** Specific target organ toxicity, repeated exposure]
Precautionary Statement Codes	P260, P262, P264, P264+P265, P270, P280, P301+P316, P301+P317, P301+P330+P331, P302+P352, P302+P361+P354, P304+P340, P305+P354+P338, P316, P317, P319, P321, P330, P361+P364, P363, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided per 321 reports by companies from 22 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

▸ European Chemicals Agency (ECHA)

8.1.2 Hazard Classes and Categories

Acute Tox. 3 (81.3%)

Acute Tox. 4 (18.7%)

Acute Tox. 3 (15%)

Skin Corr. 1A (100%)

Eye Dam. 1 (72.3%)

STOT RE 1 (69.5%)

- European Chemicals Agency (ECHA)

8.1.3 Hazards Summary

Causes burns; Inhalation may cause corrosive injuries to upper respiratory tract and lungs; Harmful by ingestion; Toxic by skin absorption; [Acros Organics MSDS] See FLUORIDES.

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

8.2 Exposure Control and Personal Protection

Exposure Summary

Biological Exposure Indices (BEI) [ACGIH] - Fluorides in urine = 2 mg/L prior to shift or 3 mg/L at end of shift; (Repeated measurements recommended.)

ACGIH - Documentation of the TLVs and BEIs, 7th Ed. Cincinnati: ACGIH Worldwide, 2020.

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

Maximum Allowable Concentration (MAK)

1.0 [mg/m3], inhalable fraction, as F (0.2 mg/m3, inhalable fraction, as Li)[German Research Foundation (DFG)]

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

8.2.1 Permissible Exposure Limit (PEL)

2.5 [mg/m3], as F

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

8.2.2 Immediately Dangerous to Life or Health (IDLH)

250.0 [mg/m3], as F

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

8.2.3 Threshold Limit Values (TLV)

2.5 [mg/m3], as F

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

8.3 Regulatory Information

The Australian Inventory of Industrial Chemicals

Chemical: Phosphate(1-), hexafluoro-, lithium

- Australian Industrial Chemicals Introduction Scheme (AICIS)

REACH Registered Substance

Status: Active Update: 02-11-2022 https://echa.europa.eu/registration-dossier/-/registered-dossier/13201

- European Chemicals Agency (ECHA)

9 Toxicity

9.1 Toxicological Information

9.1.1 Adverse Effects

Dermatotoxin - Skin burns.

Toxic Pneumonitis - Inflammation of the lungs induced by inhalation of metal fumes or toxic gases and vapors.

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

10 Literature

10.1 Consolidated References

PubChem

10.2 Springer Nature References

Springer Nature

10.3 Thieme References

Thieme Chemistry

10.4 Wiley References

Wiley

10.5 Chemical Co-Occurrences in Literature

PubChem

10.6 Chemical-Gene Co-Occurrences in Literature

PubChem

10.7 Chemical-Disease Co-Occurrences in Literature

PubChem

11 Patents

11.1 Depositor-Supplied Patent Identifiers

PubChem

Link to all deposited patent identifiers

PubChem

11.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=AXPLOJNSKRXQPA-UHFFFAOYSA-N

PATENTSCOPE (WIPO)

11.3 Chemical Co-Occurrences in Patents

PubChem

11.4 Chemical-Disease Co-Occurrences in Patents

PubChem

11.5 Chemical-Gene Co-Occurrences in Patents

PubChem

12 Classification

12.1 ChEBI Ontology

ChEBI

12.2 ChemIDplus

ChemIDplus

12.3 UN GHS Classification

GHS Classification (UNECE)

12.4 EPA CPDat Classification

EPA Chemical and Products Database (CPDat)

12.5 NORMAN Suspect List Exchange Classification

NORMAN Suspect List Exchange

12.6 EPA DSSTox Classification

- EPA DSSTox

12.7 EPA TSCA and CDR Classification

- EPA Chemicals under the TSCA

12.8 EPA Substance Registry Services Tree

- EPA Substance Registry Services

13 Information Sources

FILTER BY SOURCE

ALL SOURCES

1. ### Australian Industrial Chemicals Introduction Scheme (AICIS)

LICENSE
https://www.industrialchemicals.gov.au/copyright

Phosphate(1-), hexafluoro-, lithium

https://services.industrialchemicals.gov.au/search-inventory/

2. ### CAS Common Chemistry

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Lithium hexafluorophosphate

https://commonchemistry.cas.org/detail?cas_rn=21324-40-3

3. ### ChemIDplus

LICENSE
https://www.nlm.nih.gov/copyright.html

Lithium hexafluorophosphate

https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0021324403

ChemIDplus Chemical Information Classification

https://pubchem.ncbi.nlm.nih.gov/source/ChemIDplus

4. ### EPA Chemical Data Reporting (CDR)

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Phosphate(1-), hexafluoro-, lithium (1:1)

https://www.epa.gov/chemical-data-reporting

5. ### EPA Chemicals under the TSCA

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

Phosphate(1-), hexafluoro-, lithium (1:1)

https://www.epa.gov/chemicals-under-tsca

EPA TSCA Classification

https://www.epa.gov/tsca-inventory

6. ## EPA DSSTox

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

Phosphate(1-), hexafluoro-, lithium

https://comptox.epa.gov/dashboard/DTXSID2066698

CompTox Chemicals Dashboard Chemical Lists

https://comptox.epa.gov/dashboard/chemical-lists/

7. ## European Chemicals Agency (ECHA)

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https://echa.europa.eu/web/guest/legal-notice

Lithium hexafluorophosphate(1-)

https://chem.echa.europa.eu/100.040.289

Lithium hexafluorophosphate(1-) (EC: 244-334-7)

https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/15687

8. ## FDA Global Substance Registration System (GSRS)

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https://www.fda.gov/about-fda/about-website/website-policies#linking

LITHIUM HEXAFLUOROPHOSPHATE

https://gsrs.ncats.nih.gov/ginas/app/beta/substances/T9T8DY51J3

9. ## ChEBI

Lithium hexafluorophosphate

https://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:172376

ChEBI Ontology

http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology

10. ## EPA Chemical and Products Database (CPDat)

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

https://comptox.epa.gov/dashboard/DTXSID2066698#exposure

EPA CPDat Classification

https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat

11. Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

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https://haz-map.com/About

Lithium hexafluorophosphate

https://haz-map.com/Agents/14729

12. SpectraBase

LITHIUM HEXAFLUOROPHOSPHATE

https://spectrabase.com/spectrum/A2Tb5u13N5c

Lithium hexafluorophosphate

https://spectrabase.com/spectrum/IkAVdxlBAbj

13. Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=8051408-825419882

14. Thieme Chemistry

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https://pubchem.ncbi.nlm.nih.gov/substance/?source=22163&sourceid=8051408-825419882

15. Wikidata

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https://creativecommons.org/publicdomain/zero/1.0/

lithium hexafluorophosphate

https://www.wikidata.org/wiki/Q2583808

16. Wikipedia

Lithium hexafluorophosphate

https://en.wikipedia.org/wiki/Lithium_hexafluorophosphate

17. ## Wiley

https://pubchem.ncbi.nlm.nih.gov/substance/?source=wiley&sourceid=107920

18. PubChem

https://pubchem.ncbi.nlm.nih.gov

19. ## GHS Classification (UNECE)

GHS Classification Tree

http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

20. ## NORMAN Suspect List Exchange

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https://creativecommons.org/licenses/by/4.0/

NORMAN Suspect List Exchange Classification

https://www.norman-network.com/nds/SLE/

21. ## EPA Substance Registry Services

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

EPA SRS List Classification

https://sor.epa.gov/sor_internet/registry/substreg/LandingPage.do

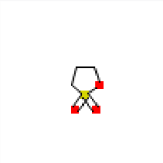
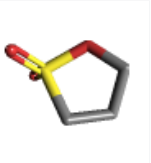
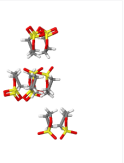
22. ## PATENTSCOPE (WIPO)

SID 403426579

https://pubchem.ncbi.nlm.nih.gov/substance/403426579

COMPOUND SUMMARY

1,3-Propane Sultone

PubChem CID	14264
Structure	 2D  3D  Crystal
Chemical Safety	Irritant Health Hazard Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_3H_6O_3S$
Synonyms	1,3-Propanesultone 1120-71-4 1,3-PROPANE SULTONE Propane sultone 1,2-oxathiolane 2,2-dioxide View More...
Molecular Weight	122.15 g/mol *Computed by PubChem 2.2 (PubChem release 2021.10.14)*
Dates	Create: 2005-03-26 Modify: 2024-10-26
Description	1,3-Propane Sultone can cause cancer according to an independent committee of scientific and health experts. California Office of Environmental Health Hazard Assessment (OEHHA)

Propane sultone appears as white crystalline solid or a colorless liquid (above 86 °F). Releases a foul odor when melting. (NIOSH, 2024)

- CAMEO Chemicals

1,3-Propane sultone is a sultone.

- ChEBI

View More...

Contents

Title and Summary

1 Structures

2 Names and Identifiers

3 Chemical and Physical Properties

4 Spectral Information

5 Related Records

6 Chemical Vendors

7 Pharmacology and Biochemistry

8 Use and Manufacturing

9 Identification

10 Safety and Hazards

11 Toxicity

12 Associated Disorders and Diseases

13 Literature

14 Patents

15 Interactions and Pathways

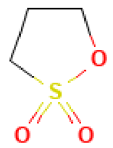
16 Biological Test Results

17 Classification

1 Structures

1.1 2D Structure

Chemical Structure Depiction

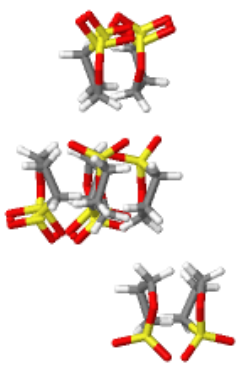


PubChem

1.2 3D Conformer

PubChem

1.3 Crystal Structures

1 of 2	View All
CCDC Number	139566
Associated Article	DOI:10.1107/S0108270199011592
Crystal Structure Data	DOI:10.5517/cc4p745
Crystal Structure Depiction	

The Cambridge Structural Database

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

oxathiolane 2,2-dioxide

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

PubChem

2.1.2 InChI

InChI=1S/C3H6O3S/c4-7(5)3-1-2-6-7/h1-3H2

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

- **PubChem**

2.1.3 InChIKey

FSSPGSAQUIYDCN-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

- **PubChem**

2.1.4 SMILES

C1COS(=O)(=O)C1

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

- **PubChem**

2.2 Molecular Formula

$C_3H_6O_3S$

Computed by PubChem 2.2 (PubChem release 2021.10.14)

- **Australian Industrial Chemicals Introduction Scheme (AICIS); CAMEO Chemicals; PubChem**

$C_3H_6O_3S$

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

2.3 Other Identifiers

2.3.1 CAS

1120-71-4

- Australian Industrial Chemicals Introduction Scheme (AICIS); CAMEO Chemicals; CAS Common C...

2.3.2 European Community (EC) Number

214-317-9

- European Chemicals Agency (ECHA)

2.3.3 UNII

L6NTK7VJX9

- FDA Global Substance Registration System (GSRS)

2.3.4 UN Number

2810 (PROPANE SULTONE)

- CAMEO Chemicals

2811

- ILO-WHO International Chemical Safety Cards (ICSCs)

3077

- NJDOH RTK Hazardous Substance List

2.3.5 ChEBI ID

CHEBI:82370

- ChEBI

2.3.6 ChEMBL ID

CHEMBL3185243

- ChEMBL

2.3.7 DSSTox Substance ID

DTXSID8021195

- EPA DSSTox

2.3.8 HMDB ID

HMDB0244180

- Human Metabolome Database (HMDB)

2.3.9 ICSC Number

1524

- ILO-WHO International Chemical Safety Cards (ICSCs)

2.3.10 KEGG ID

C19296

- KEGG

2.3.11 NCI Thesaurus Code

C44437

- NCI Thesaurus (NCIt)

2.3.12 Nikkaji Number

J4.528D

- Japan Chemical Substance Dictionary (Nikkaji)

J778.863K

- Japan Chemical Substance Dictionary (Nikkaji)

2.3.13 NSC Number

42386

- DTP/NCI

2.3.14 RTECS Number

RP5425000

- The National Institute for Occupational Safety and Health (NIOSH)

2.3.15 Wikidata

Q1933902

- Wikidata

2.3.16 Wikipedia

Alfetamine

- Wikipedia

1,3-Propane_sultone

- Wikipedia

2.4 Synonyms

2.4.1 MeSH Entry Terms

1,3-propane sultone
propane sultone

- Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

1,3-Propanesultone	RCRA waste number U193	DTXSID8021195
1120-71-4	CCRIS 535	3-Hydroxy-1-propan
1,3-PROPANE SULTONE	NSC 42386	1,3-TRIMETHYLENE S
Propane sultone	1,2-Oxathrolane 2,2-dioxide	AI3-26990
1,2-oxathiolane 2,2-dioxide	HSDB 1673	MFCD00005355
1,2-Oxathiolane, 2,2-dioxide	UNII-L6NTK7VJX9	NSC-42386
Propanesultone	L6NTK7VJX9	3-Hydroxy-1-propan
oxathiolane 2,2-dioxide	EINECS 214-317-9	DTXCID001195
PROPYL SULTONE	3-Hydroxy-1-propanesulfonic acid gamma-sultone	CHEBI:82370
.gamma.-Propane sultone	BRN 0109782	EC 214-317-9

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	122.15 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
XLogP3-AA	-0.2	Computed by XLogP3 3.0 (PubChem release 2021.10.14)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Hydrogen Bond Acceptor Count	3	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Rotatable Bond Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Exact Mass	122.00376522 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Monoisotopic Mass	122.00376522 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)

Topological Polar Surface Area	51.8Å^2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Heavy Atom Count	7	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	140	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.10.14)

PubChem

3.2 Experimental Properties

3.2.1 Physical Description

Propane sultone appears as white crystalline solid or a colorless liquid (above 86 °F). Releases a foul odor when melting. (NIOSH, 2024)

CAMEO Chemicals

White, crystalline solid or a colorless liquid (above 86 degrees F). [Note: Releases a foul odor as it melts.]; [NIOSH]

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

WHITE CRYSTALS OR COLOURLESS LIQUID WITH CHARACTERISTIC ODOUR.

- ILO-WHO International Chemical Safety Cards (ICSCs)

White, crystalline solid or a colorless liquid (above 86 °F). [Note: Releases a foul odor as it melts.]

- The National Institute for Occupational Safety and Health (NIOSH)

3.2.2 Color / Form

COLORLESS LIQ OR WHITE CRYSTALS

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 253 (1974)*

- Hazardous Substances Data Bank (HSDB)

White, crystalline solid or a colorless liquid (above 86 degrees F).

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 94-116. Washington, D.C.: U.S. Government Printing Office, June 1994., p. 264

- Hazardous Substances Data Bank (HSDB)

3.2.3 Odor

Foul odor above 31.11 °C.

American Conference of Governmental Industrial Hygienists. TLV's Threshold Limit Values for Chemical Substances in Workroom Air Adopted by ACGIH for 1980. Cincinnati, Ohio: ACGIH, 1980., p. 346

- Hazardous Substances Data Bank (HSDB)

Releases a fould odor as it melts.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 94-116. Washington, D.C.: U.S. Government Printing Office, June 1994., p. 264

- Hazardous Substances Data Bank (HSDB)

3.2.4 Boiling Point

180 °C at 0.039 atm.

American Conference of Governmental Industrial Hygienists. TLV's Threshold Limit Values for Chemical Substances in Workroom Air Adopted by ACGIH for 1980. Cincinnati, Ohio: ACGIH, 1980., p. 346

- Hazardous Substances Data Bank (HSDB)

3.2.5 Melting Point

86 °F (NIOSH, 2024)

- CAMEO Chemicals

31 °C

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 253 (1974)*

- Hazardous Substances Data Bank (HSDB); ILO-WHO International Chemical Safety Cards (ICSCs)

86 °F

- The National Institute for Occupational Safety and Health (NIOSH)

3.2.6 Flash Point

greater than 235 °F (NIOSH, 2024)

- CAMEO Chemicals

Flash point > 235 °F

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

>110 °C

- ILO-WHO International Chemical Safety Cards (ICSCs)

>235 °F

- The National Institute for Occupational Safety and Health (NIOSH)

3.2.7 Solubility

10 % (NIOSH, 2024)

- CAMEO Chemicals

READILY SOL IN KETONES, ESTERS & AROMATIC HYDROCARBONS

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 253 (1974)*

- **Hazardous Substances Data Bank (HSDB)**

INSOL IN ALIPHATIC HYDROCARBONS

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 253 (1974)*

- **Hazardous Substances Data Bank (HSDB)**

SOL IN WATER (100 G/L)

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 253 (1974)*

- **Hazardous Substances Data Bank (HSDB)**

Solubility in water, g/100ml: 10 (moderate)

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

10%

- **The National Institute for Occupational Safety and Health (NIOSH)**

3.2.8 Density

1.39 (NIOSH, 2024) - Denser than water; will sink

- **CAMEO Chemicals**

SPECIFIC GRAVITY: 1.393 @ 40 °C/4 °C

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 253 (1974)*

- **Hazardous Substances Data Bank (HSDB)**

Density (at 25 °C): 1.392 g/cm^3

- ILO-WHO International Chemical Safety Cards (ICSCs)

1.39

- The National Institute for Occupational Safety and Health (NIOSH)

3.2.9 Vapor Pressure

0.27 [mmHg]

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

3.2.10 Refractive Index

INDEX OF REFRACTION: 1.450 @ 40 °C/D

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 253 (1974)*

- Hazardous Substances Data Bank (HSDB)

3.2.11 Other Experimental Properties

HYDROLYZES TO 3-HYDROXY-1-PROPANESULFONIC ACID.

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 253 (1974)*

- Hazardous Substances Data Bank (HSDB)

3.3 SpringerMaterials Properties

Dielectric constant
Fusion temperature
Melting temperature
Optical coefficient
Phase transition
Refractive index
Transition enthalpy

Viscosity

- SpringerMaterials

3.4 Chemical Classes

Other Classes -> Sulfur Compounds

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

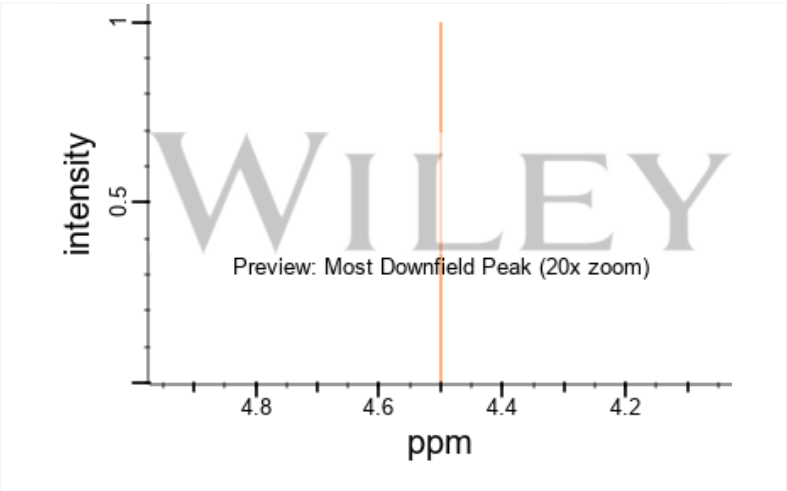
4 Spectral Information

4.1 1D NMR Spectra

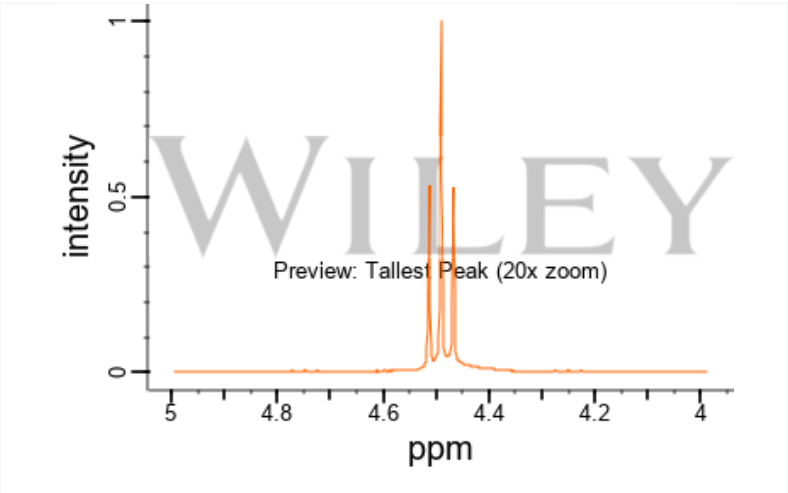
1D NMR Spectra	NMR: 10:14C (Aldrich Library of Mass Spectra, Aldrich Chemical Co, Milwaukee, WI)

- Hazardous Substances Data Bank (HSDB)

4.1.1 1H NMR Spectra

1 of 2	
Instrument Name	Varian A-60D
Copyright	Copyright © 2009-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

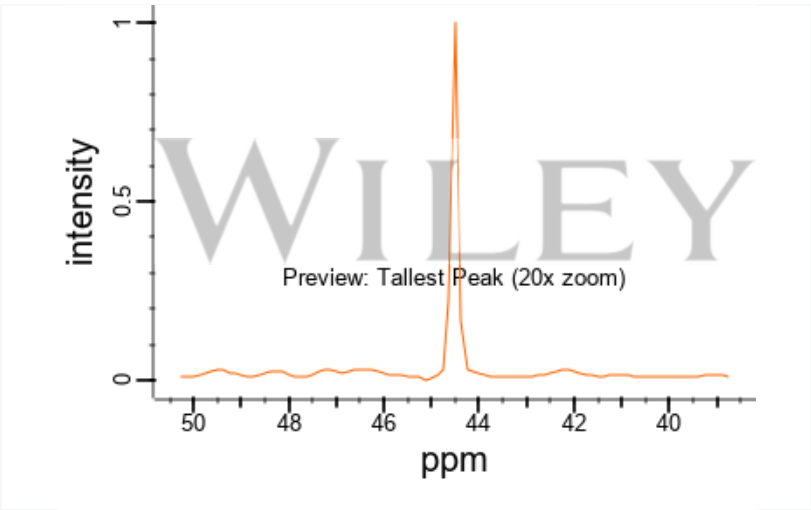
SpectraBase

2 of 2	
Source of Spectrum	Sigma-Aldrich Co. LLC.
Source of Sample	Sigma-Aldrich Co. LLC.
Catalog Number	P50706
Copyright	Copyright © 2021-2024 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

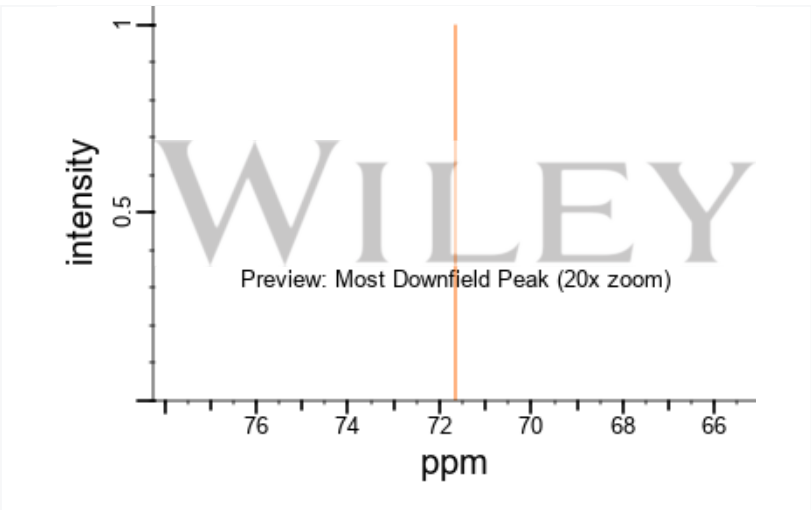
SpectraBase

4.1.2 13C NMR Spectra

1 of 2	
Source of Sample	Tokyo Kasei Koygo Company, Ltd., Tokyo, Japan
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail	

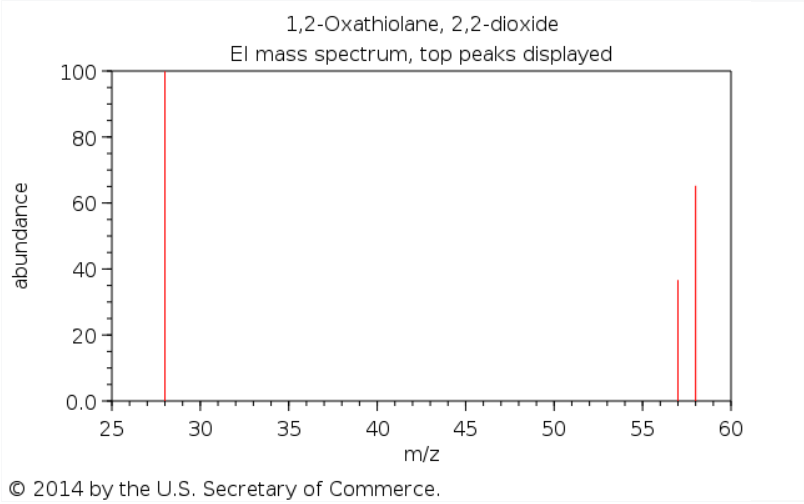
SpectraBase

2 of 2	
Instrument Name	Bruker WP-80
Copyright	Copyright © 2002-2024 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
Thumbnail	

SpectraBase

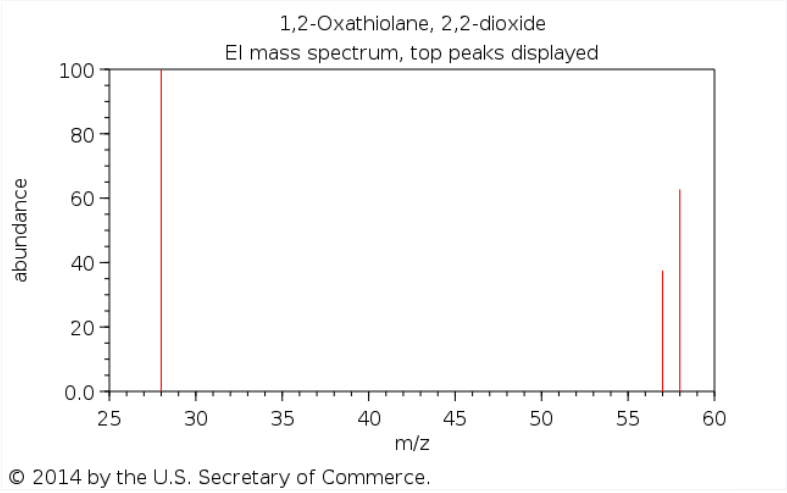
4.2 Mass Spectrometry

4.2.1 GC-MS

1 of 4	View All
NIST Number	230303
Library	Main library
Total Peaks	70
m/z Top Peak	28
m/z 2nd Highest	58
m/z 3rd Highest	57
Thumbnail	

NIST Mass Spectrometry Data Center

2 of 4	View All
NIST Number	157174
Library	Replicate library
Total Peaks	54
m/z Top Peak	28
m/z 2nd Highest	58
m/z 3rd Highest	57

Thumbnail	

NIST Mass Spectrometry Data Center

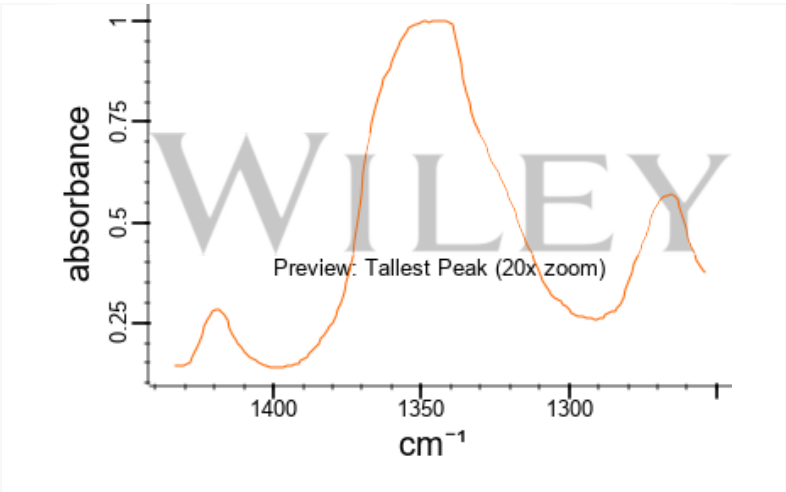
4.3 IR Spectra

IR Spectra	IR: 2:479A (Aldrich Library of Infrared Spectra, Aldrich Chemical Co, Milwaukee, WI)

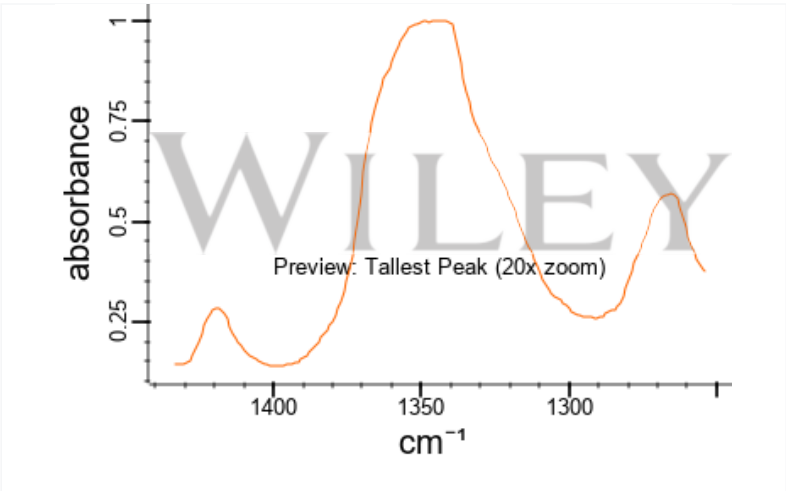
Hazardous Substances Data Bank (HSDB)

4.3.1 FTIR Spectra

1 of 2	
Technique	CAPILLARY CELL: MELT
Source of Sample	Aldrich Chemical Company, Inc., Milwaukee, Wisconsin
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.

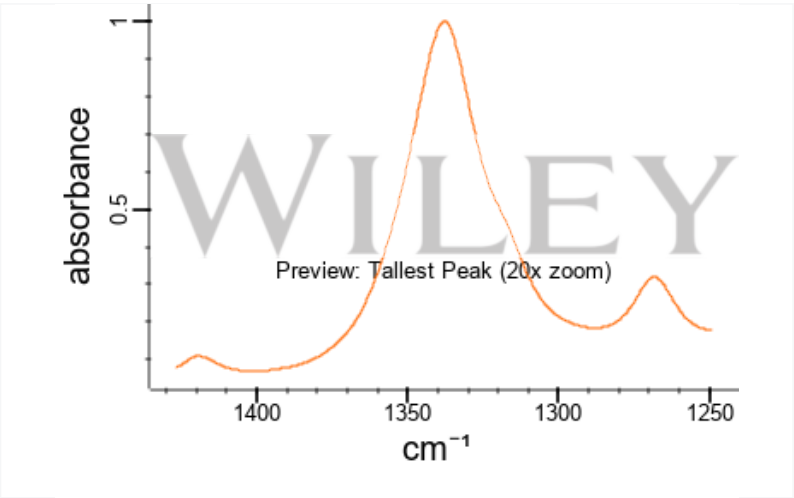
Thumbnail	

SpectraBase

2 of 2	
Technique	CAPILLARY CELL: MELT
Source of Sample	ALDRICH CHEMICAL COMPANY, INC., MILWAUKEE, WISCONSIN
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

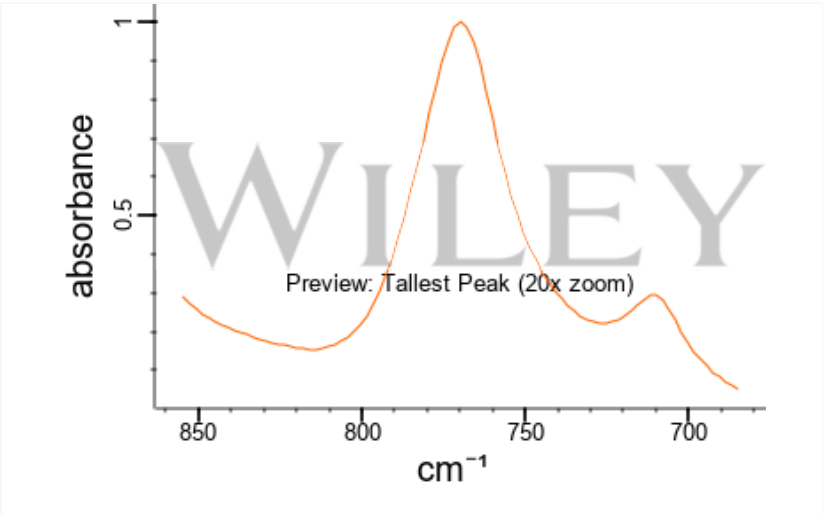
SpectraBase

4.3.2 ATR-IR Spectra

1 of 2	
Instrument Name	PerkinElmer SpectrumTwo
Technique	ATR-IR
Copyright	Copyright © 2016-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

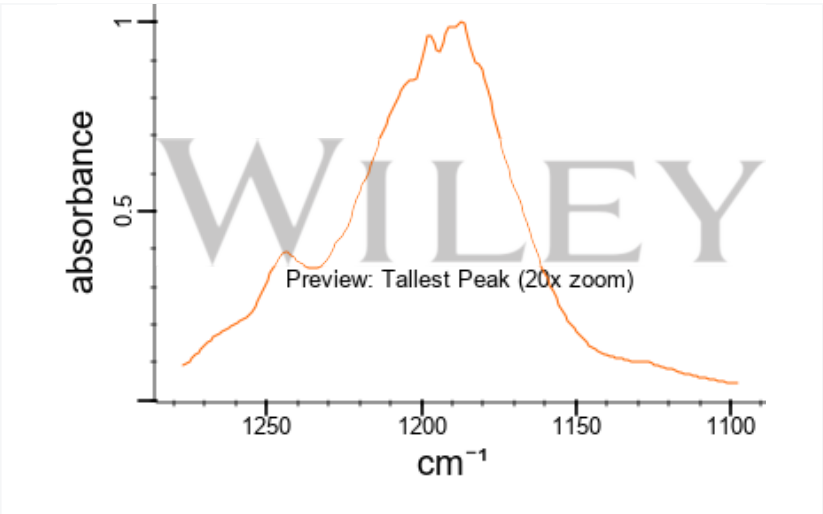
SpectraBase

2 of 2	
Source of Sample	Aldrich
Catalog Number	291250
Copyright	Copyright © 2018-2024 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2018-2024 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail	

▸ SpectraBase

4.3.3 Vapor Phase IR Spectra

Instrument Name	DIGILAB FTS-14
Technique	Vapor Phase
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

▸ SpectraBase

5 Related Records

5.1 Related Compounds with Annotation

Follow these links to do a live 2D search or do a live 3D search for this compound, sorted by annotation score. This section is deprecated (see here for details), but these live search links provide equivalent functionality to the table that was previously shown here.

PubChem

5.2 Related Compounds

Same Connectivity Count	2
Same Parent, Connectivity Count	11
Same Parent, Exact Count	10
Mixtures, Components, and Neutralized Forms Count	534
Similar Compounds (2D)	View in PubChem Search
Similar Conformers (3D)	View in PubChem Search

PubChem

5.3 Substances

5.3.1 PubChem Reference Collection SID

500716324

PubChem

5.3.2 Related Substances

All Count	732
Same Count	171
Mixture Count	561

PubChem

5.3.3 Substances by Category

PubChem

5.4 Entrez Crosslinks

PubMed Count	34
Taxonomy Count	1
Gene Count	1

PubChem

5.5 NCBI LinkOut

NCBI

6 Chemical Vendors

PubChem

7 Pharmacology and Biochemistry

7.1 Biological Half-Life

HALF-LIFE IS 110 MIN AT 37 °C IN **PHOSPHATE** BUFFER.

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 253 (1974)*

- **Hazardous Substances Data Bank (HSDB)**

7.2 Mechanism of Action

The reaction of propane sultone with **guanosine** and DNA at pH 6-7.5 gave an N7-alkylguanosine as the main products (>90%). Similar evidence suggested that 2 of the minor adducts were N1-and 6-alkyl derivatives, accounting for approx 1.6% and 0.5% of the total adduct,/respectively/. N7- and N1-alkylguanine were also detected in the DNA reacted with propane sultone.

PMID:6872144

Hemminki K; Carcinogenesis 4 (7): 901-4 (1983)

- **Hazardous Substances Data Bank (HSDB)**

8 Use and Manufacturing

8.1 Uses

1,3-Propane sultone is used as a chemical intermediate to introduce sulfopropyl groups into molecules and to confer **water** solubility and anionic character.

- **EPA Air Toxics**

Sources/Uses

Used as a chemical intermediate in the production of organic chemicals; [HSDB]

- **Haz-Map, Information on Hazardous Chemicals and Occupational Diseases**

1,3-PROPANE SULTONE IS USED AS CHEMICAL INTERMEDIATE TO INTRODUCE SULFOPROPYL GROUP ... INTO MOLECULES, & TO CONFER **WATER** SOLUBILITY & ANIONIC CHARACTER.

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 254 (1974)*

- **Hazardous Substances Data Bank (HSDB)**

CHEM INT, EG, A SULFOALKYLATING AGENT (FORMER USE)

SRI

- **Hazardous Substances Data Bank (HSDB)**

8.1.1 Use Classification

Hazardous Air Pollutants (HAPs)

- **EPA Air Toxics**

Hazard Classes and Categories -> Carcinogens, Mutagens, Flammable - 2nd degree

- **NJDOH RTK Hazardous Substance List**

8.2 Methods of Manufacturing

PREPN: 1,3-PROPANE SULTONE IS PRODUCED COMMERCIALLY BY DEHYDRATING GAMMA-HYDROXY-PROPANESULFONIC ACID, WHICH IS PREPARED FROM SODIUM HYDROXYPROPANESULFONATE. THIS **SODIUM** SALT IS PREPARED BY ADDITION OF **SODIUM BISULFITE** TO **ALLYL ALCOHOL**.

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 254 (1974)*

- **Hazardous Substances Data Bank (HSDB)**

8.3 Formulations / Preparations

Commercial grade contains 99% active ingredient, 0.2% **water** and 0.8% acid (as 3-hydroxy-1-propanesulphonic acid)

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 254 (1974)*

- **Hazardous Substances Data Bank (HSDB)**

8.4 General Manufacturing Information

EPA TSCA Commercial Activity Status

1,2-Oxathiolane, 2,2-dioxide: ACTIVE

- EPA Chemicals under the TSCA

8.5 Sampling Procedures

Analyte: 1,3-propane sultone; procedure: adsorption onto the walls of a separation tube; flow rate 330 ml/min.

Royal Society of Chemistry. Measurement Techniques for Carcinogenic Agents in Workplace Air. Publ. No. EUR 11897, Commission of the European Communities/Scientific and Technical Communication Unit, Luxembourg. Great Britian: St. Edmundsbury Press Ltd, 1989., p. 27

- Hazardous Substances Data Bank (HSDB)

9 Identification

9.1 Analytic Laboratory Methods

Analyte: 1,3-propane sultone; Procedure; High-pressure liquid chromatography; range 1 to 16 ug; overall precision: 6 percent at 4 ug; Limit of detection 0.5 ug; interference: none recorded.

Royal Society of Chemistry. Measurement Techniques for Carcinogenic Agents in Workplace Air. Publ. No. EUR 11897, Commission of the European Communities/Scientific and Technical Communication Unit, Luxembourg. Great Britian: St. Edmundsbury Press Ltd, 1989., p. 27

- Hazardous Substances Data Bank (HSDB)

10 Safety and Hazards

10.1 Hazards Identification

10.1.1 GHS Classification

1 of 6 View All

Pictogram(s)

Corrosive Acute Toxic Irritant Health Hazard

Signal	Danger
GHS Hazard Statements	H301 (62.6%): Toxic if swallowed [**Danger** Acute toxicity, oral] H302 (37.4%): Harmful if swallowed [**Warning** Acute toxicity, oral] H311 (62.2%): Toxic in contact with skin [**Danger** Acute toxicity, dermal] H312 (37.8%): Harmful in contact with skin [**Warning** Acute toxicity, dermal] H315 (62.2%): Causes skin irritation [**Warning** Skin corrosion/irritation] H318 (62.2%): Causes serious eye damage [**Danger** Serious eye damage/eye irritation] H319 (18%): Causes serious eye irritation [**Warning** Serious eye damage/eye irritation] H332 (62.2%): Harmful if inhaled [**Warning** Acute toxicity, inhalation] H341 (62.2%): Suspected of causing genetic defects [**Warning** Germ cell mutagenicity] H350 (100%): May cause cancer [**Danger** Carcinogenicity] H412 (39.2%): Harmful to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]
Precautionary Statement Codes	P203, P261, P262, P264, P264+P265, P270, P271, P273, P280, P301+P316, P301+P317, P302+P352, P304+P340, P305+P351+P338, P305+P354+P338, P316, P317, P318, P321, P330, P332+P317, P337+P317, P361+P364, P362+P364, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided per 222 reports by companies from 11 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

▸ European Chemicals Agency (ECHA)

10.1.2 Hazard Classes and Categories

Acute Tox. 3 (62.6%)

Acute Tox. 4 (37.4%)

Acute Tox. 3 (62.2%)

Acute Tox. 4 (37.8%)

Skin Irrit. 2 (62.2%)

Eye Dam. 1 (62.2%)

Eye Irrit. 2 (18%)

Acute Tox. 4 (62.2%)

Muta. 2 (62.2%)

Carc. 1B (100%)

Aquatic Chronic 3 (39.2%)

- European Chemicals Agency (ECHA)

Carcinogenicity - category 1B

Germ cell mutagenicity - category 2

Eye damage - category 1

Skin irritation - category 2

Acute toxicity (ingestion) - category 3

Acute toxicity (dermal) - category 3

Acute toxicity (inhalation) - category 2

- Hazardous Chemical Information System (HCIS), Safe Work Australia

View More...

10.1.3 Health Hazards

Excerpt from NIOSH Pocket Guide for Propane sultone:

Exposure Routes: Inhalation, skin absorption, ingestion, skin and/or eye contact

Symptoms: Irritation eyes, skin, respiratory system; [potential occupational carcinogen]

Target Organs: Eyes, skin, respiratory system

Cancer Site: [in animals: skin tumors, leukemia, gliomas] (NIOSH, 2024)

- CAMEO Chemicals

10.1.4 Fire Hazards

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]:

Combustible material: may burn but does not ignite readily. When heated, vapors may form explosive mixtures with air: indoors, outdoors and sewers explosion hazards. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Corrosives in contact with metals may evolve flammable **hydrogen** gas. Containers may explode when

heated. Runoff may pollute waterways. Substance may be transported in a molten form. (ERG, 2024)

2024 Emergency Response Guidebook, ***https://www.phmsa.dot.gov/training/hazmat/erg/emergency-response-guidebook-erg***

- CAMEO Chemicals

Gives off irritating or toxic fumes (or gases) in a fire.

- ILO-WHO International Chemical Safety Cards (ICSCs)

10.1.5 Hazards Summary

1,3-Propane sultone is used as a chemical intermediate. No information is available on the acute (short- term), chronic (long-term), reproductive, developmental, and carcinogenic effects of 1,3-propane sultone in humans. In rodents exposed to 1,3-propane sultone via gavage (experimentally placing the chemical in the stomach) and intravenous injection, tumors of the brain and other central nervous system (CNS) tissues have been observed. Leukemia, and tumors of the ear duct, small intestine, kidneys, lung, mammary gland, uterus, and skin have been reported in rodents exposed via gavage, injection, or dermal contact. The International Agency for Research on Cancer (IARC) has classified 1,3-propane sultone as a Group 2B, possible human carcinogen.

- EPA Air Toxics

A carcinogen in animal testing; [HSDB]

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

10.1.6 EPA Hazardous Waste Number

U193; A toxic waste when a discarded commercial chemical product or manufacturing chemical intermediate or an off-specification commercial chemical product or manufacturing chemical intermediate.

- Hazardous Substances Data Bank (HSDB)

10.2 Safety and Hazard Properties

10.2.1 Flammable Limits

Flammability

Combustible Solid

- The National Institute for Occupational Safety and Health (NIOSH)

10.2.2 NIOSH Recommendations

NIOSH considers propane sultone to be a potential occupational carcinogen.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 264

- Hazardous Substances Data Bank (HSDB)

NIOSH usually recommends that occupational exposures to carcinogens be limited to the lowest feasible concentration.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 264

- Hazardous Substances Data Bank (HSDB)

10.3 First Aid Measures

Inhalation First Aid

Fresh air, rest.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Skin First Aid

Wear protective gloves when administering first aid. Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer for medical attention if skin irritation occurs.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Eye First Aid

Rinse with plenty of water for several minutes (remove contact lenses if easily possible). Refer for medical attention.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Ingestion First Aid

Rinse mouth. Seek medical attention if you feel unwell.

- ILO-WHO International Chemical Safety Cards (ICSCs)

10.3.1 First Aid

Excerpt from NIOSH Pocket Guide for Propane sultone:

Eye: IRRIGATE IMMEDIATELY - If this chemical contacts the eyes, immediately wash (irrigate) the eyes with large amounts of water, occasionally lifting the lower and upper lids. Get medical attention immediately.

Skin: WATER FLUSH IMMEDIATELY - If this chemical contacts the skin, immediately flush the contaminated skin with water. If this chemical penetrates the clothing, immediately remove the clothing and flush the skin with water. Get medical attention promptly.

Breathing: RESPIRATORY SUPPORT - If a person breathes large amounts of this chemical, move the exposed person to fresh air at once. If breathing has stopped, perform artificial respiration. Keep the affected person warm and at rest. Get medical attention as soon as possible.

Swallow: MEDICAL ATTENTION IMMEDIATELY - If this chemical has been swallowed, get medical attention immediately. (NIOSH, 2024)

- CAMEO Chemicals

(See general first aid procedures)

Eye: Irrigate immediately - If this chemical contacts the eyes, immediately wash (irrigate) the eyes with large amounts of water, occasionally lifting the lower and upper lids. Get medical attention immediately.

Skin: Water flush immediately - If this chemical contacts the skin, immediately flush the contaminated skin with water. If this chemical penetrates the clothing, immediately remove the clothing and flush the skin with water. Get medical attention promptly.

Breathing: Respiratory support

Swallow: Medical attention immediately - If this chemical has been swallowed, get medical attention immediately.

- The National Institute for Occupational Safety and Health (NIOSH)

10.4 Fire Fighting

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]:

SMALL FIRE: Dry chemical, CO2 or water spray.

LARGE FIRE: Dry chemical, CO2, alcohol-resistant foam or **water** spray. If it can be done safely, move undamaged containers away from the area around the fire. Dike runoff from fire control for later disposal.

FIRE INVOLVING TANKS, RAIL TANK CARS OR HIGHWAY TANKS: Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles. Do not get **water** inside containers. Cool containers with flooding quantities of **water** until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks in direct contact with flames. (ERG, 2024)

2024 Emergency Response Guidebook, ***https://www.phmsa.dot.gov/training/hazmat/erg/emergency-response-guidebook-erg***

- **CAMEO Chemicals**

In case of fire in the surroundings, use appropriate extinguishing media.

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

10.5 Accidental Release Measures

10.5.1 Isolation and Evacuation

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]:

IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids.

SPILL: Increase the immediate precautionary measure distance, in the downwind direction, as necessary.

FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

2024 Emergency Response Guidebook, ***https://www.phmsa.dot.gov/training/hazmat/erg/emergency-response-guidebook-erg***

- **CAMEO Chemicals**

10.5.2 Spillage Disposal

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Vacuum with specialist equipment or carefully sweep into sealable containers. If appropriate, moisten first to prevent dusting. If liquid: collect leaking liquid in sealable

containers as far as possible. Carefully collect remainder. Then store and dispose of according to local regulations.

- ILO-WHO International Chemical Safety Cards (ICSCs)

10.5.3 Cleanup Methods

PRECAUTIONS FOR "CARCINOGENS": A high-efficiency particulate arrestor (HEPA) or charcoal filters can be used to minimize amt of carcinogen in exhausted air ventilated safety cabinets, lab hoods, glove boxes or animal rooms ... Filter housing that is designed so that used filters can be transferred into plastic bag without contaminating maintenance staff is avail commercially. Filters should be placed in plastic bags immediately after removal ... The plastic bag should be sealed immediately ... The sealed bag should be labelled properly ... Waste liquids ... should be placed or collected in proper containers for disposal. The lid should be secured & the bottles properly labelled. Once filled, bottles should be placed in plastic bag, so that outer surface ... is not contaminated ... The plastic bag should also be sealed & labelled. ... Broken glassware ... should be decontaminated by solvent extraction, by chemical destruction, or in specially designed incinerators. /Chemical Carcinogens/

Montesano, R., H. Bartsch, E.Boyland, G. Della Porta, L. Fishbein, R. A. Griesemer, A.B. Swan, L. Tomatis, and W. Davis (eds.). Handling Chemical Carcinogens in the Laboratory: Problems of Safety. IARC Scientific Publications No. 33. Lyon, France: International Agency for Research on Cancer, 1979., p. 15

- Hazardous Substances Data Bank (HSDB)

10.5.4 Disposal Methods

Generators of waste (equal to or greater than 100 kg/mo) containing this contaminant, EPA hazardous waste number U193, must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.

40 CFR 240-280, 300-306, 702-799 (7/1/89)

- Hazardous Substances Data Bank (HSDB)

A potential candidate for rotary kiln incineration at a temperature range of 820 to 1,600 °C and residence times of seconds for liquids and gases, and hours for solids. A potential candidate for fluidized bed incineration at a temperature range of 450 to 980 °C and residence times of seconds for liquids and gases, and longer for solids.

USEPA; Engineering Handbook for Hazardous Waste Incineration p.3-15 (1981) EPA 68-03-3025

- Hazardous Substances Data Bank (HSDB)

Dissolve or mix propane sultone with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Aldrich; Catalog Hdbk Fine Chem p.927 (1984)

- **Hazardous Substances Data Bank (HSDB)**

PRECAUTIONS FOR "CARCINOGENS": There is no universal method of disposal that has been proved satisfactory for all carcinogenic compounds & specific methods of chem destruction ... published have not been tested on all kinds of carcinogen-containing waste. ... summary of avail methods & recommendations ... /given/ must be treated as guide only. /Chemical Carcinogens/

Montesano, R., H. Bartsch, E.Boyland, G. Della Porta, L. Fishbein, R. A. Griesemer, A.B. Swan, L. Tomatis, and W. Davis (eds.). Handling Chemical Carcinogens in the Laboratory: Problems of Safety. IARC Scientific Publications No. 33. Lyon, France: International Agency for Research on Cancer, 1979., p. 14

- **Hazardous Substances Data Bank (HSDB)**

For more Disposal Methods (Complete) data for 1,3-PROPANE SULTONE (8 total), please visit the **HSDB record page**.

- **Hazardous Substances Data Bank (HSDB)**

10.5.5 Preventive Measures

PRECAUTIONS FOR "CARCINOGENS": Smoking, drinking, eating, storage of food or of food & beverage containers or utensils, & the application of cosmetics should be prohibited in any laboratory. All personnel should remove gloves, if worn, after completion of procedures in which carcinogens have been used. They should ... wash ... hands, preferably using dispensers of liq detergent, & rinse ... thoroughly. Consideration should be given to appropriate methods for cleaning the skin, depending on nature of the contaminant. No standard procedure can be recommended, but the use of organic solvents should be avoided. Safety pipettes should be used for all pipetting. /Chemical Carcinogens/

Montesano, R., H. Bartsch, E.Boyland, G. Della Porta, L. Fishbein, R. A. Griesemer, A.B. Swan, L. Tomatis, and W. Davis (eds.). Handling Chemical Carcinogens in the Laboratory: Problems of Safety. IARC Scientific Publications No. 33. Lyon, France: International Agency for Research on Cancer, 1979., p. 8

- **Hazardous Substances Data Bank (HSDB)**

PRECAUTIONS FOR "CARCINOGENS": In animal laboratory, personnel should remove their outdoor clothes & wear protective suits (preferably disposable, one-piece & close-fitting at ankles & wrists), gloves, hair covering & overshoes. ... clothing should be changed daily but ... discarded immediately if obvious contamination occurs ... /also,/ workers should shower

immediately. In chemical laboratory, gloves & gowns should always be worn ... however, gloves should not be assumed to provide full protection. Carefully fitted masks or respirators may be necessary when working with particulates or gases, & disposable plastic aprons might provide addnl protection. If gowns are of distinctive color, this is a reminder that they should not be worn outside of lab. /Chemical Carcinogens/

Montesano, R., H. Bartsch, E.Boyland, G. Della Porta, L. Fishbein, R. A. Griesemer, A.B. Swan, L. Tomatis, and W. Davis (eds.). Handling Chemical Carcinogens in the Laboratory: Problems of Safety. IARC Scientific Publications No. 33. Lyon, France: International Agency for Research on Cancer, 1979., p. 8

Hazardous Substances Data Bank (HSDB)

PRECAUTIONS FOR "CARCINOGENS": ... Operations connected with synth & purification ... should be carried out under well-ventilated hood. Analytical procedures ... should be carried out with care & vapors evolved during ... procedures should be removed. ... Expert advice should be obtained before existing fume cupboards are used ... & when new fume cupboards are installed. It is desirable that there be means for decreasing the rate of air extraction, so that carcinogenic powders can be handled without ... powder being blown around the hood. Glove boxes should be kept under negative air pressure. Air changes should be adequate, so that concn of vapors of volatile carcinogens will not occur. /Chemical Carcinogens/

Montesano, R., H. Bartsch, E.Boyland, G. Della Porta, L. Fishbein, R. A. Griesemer, A.B. Swan, L. Tomatis, and W. Davis (eds.). Handling Chemical Carcinogens in the Laboratory: Problems of Safety. IARC Scientific Publications No. 33. Lyon, France: International Agency for Research on Cancer, 1979., p. 8

Hazardous Substances Data Bank (HSDB)

PRECAUTIONS FOR "CARCINOGENS": Vertical laminar-flow biological safety cabinets may be used for containment of in vitro procedures ... provided that the exhaust air flow is sufficient to provide an inward air flow at the face opening of the cabinet, & contaminated air plenums that are under positive pressure are leak-tight. Horizontal laminar-flow hoods or safety cabinets, where filtered air is blown across the working area towards the operator, should never be used ... Each cabinet or fume cupboard to be used ... should be tested before work is begun (eg, with fume bomb) & label fixed to it, giving date of test & avg air-flow measured. This test should be repeated periodically & after any structural changes. /Chemical Carcinogens/

Montesano, R., H. Bartsch, E.Boyland, G. Della Porta, L. Fishbein, R. A. Griesemer, A.B. Swan, L. Tomatis, and W. Davis (eds.). Handling Chemical Carcinogens in the Laboratory: Problems of Safety. IARC Scientific Publications No. 33. Lyon, France: International Agency for Research on Cancer, 1979., p. 9

Hazardous Substances Data Bank (HSDB)

For more Preventive Measures (Complete) data for 1,3-PROPANE SULTONE (13 total), please visit the **HSDB record page**.

- Hazardous Substances Data Bank (HSDB)

10.6 Handling and Storage

10.6.1 Nonfire Spill Response

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]:

ELIMINATE all ignition sources (no smoking, flares, sparks or flames) from immediate area. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Stop leak if you can do it without risk. Prevent entry into waterways, sewers, basements or confined areas. Absorb or cover with dry earth, sand or other non-combustible material and transfer to containers. DO NOT GET **WATER** INSIDE CONTAINERS. (ERG, 2024)

*2024 Emergency Response Guidebook, **https://www.phmsa.dot.gov/training/hazmat/erg/emergency-response-guidebook-erg***

- CAMEO Chemicals

10.6.2 Safe Storage

Dry. Well closed. Separated from food and feedstuffs.

- ILO-WHO International Chemical Safety Cards (ICSCs)

10.6.3 Storage Conditions

PRECAUTIONS FOR "CARCINOGENS": Storage site should be as close as practical to lab in which carcinogens are to be used, so that only small quantities required for ... expt need to be carried. Carcinogens should be kept in only one section of cupboard, an explosion-proof refrigerator or freezer (depending on chemicophysical properties ...) that bears appropriate label. An inventory ... should be kept, showing quantity of carcinogen & date it was acquired ... Facilities for dispensing ... should be contiguous to storage area. /Chemical Carcinogens/

Montesano, R., H. Bartsch, E.Boyland, G. Della Porta, L. Fishbein, R. A. Griesemer, A.B. Swan, L. Tomatis, and W. Davis (eds.). Handling Chemical Carcinogens in the Laboratory: Problems of Safety. IARC Scientific Publications No. 33. Lyon, France: International Agency for Research on Cancer, 1979., p. 13

- Hazardous Substances Data Bank (HSDB)

10.7 Exposure Control and Personal Protection

10.7.1 Recommended Exposure Limit (REL)

Ca See Appendix A

- The National Institute for Occupational Safety and Health (NIOSH)

10.7.2 Permissible Exposure Limit (PEL)

none

- The National Institute for Occupational Safety and Health (NIOSH)

10.7.3 Immediately Dangerous to Life or Health (IDLH)

A potential occupational carcinogen. (NIOSH, 2024)

- CAMEO Chemicals

NIOSH considers propane sultone to be a potential occupational carcinogen.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 264

- Hazardous Substances Data Bank (HSDB)

Ca [N.D.]

See: IDLH INDEX

- The National Institute for Occupational Safety and Health (NIOSH)

10.7.4 Threshold Limit Values (TLV)

Exposure by all routes should be carefully controlled to levels as low as possible.

American Conference of Governmental Industrial Hygienists TLVs and BEIs. Threshold Limit Values for Chemical Substances and Physical Agents and Biological Exposure Indices. Cincinnati, OH, 2008, p. 49

- Hazardous Substances Data Bank (HSDB)

A3; Confirmed animal carcinogen with unknown relevance to humans.

American Conference of Governmental Industrial Hygienists TLVs and BEIs. Threshold Limit Values for Chemical Substances and Physical Agents and Biological Exposure Indices. Cincinnati, OH, 2008, p. 49

- Hazardous Substances Data Bank (HSDB)

A3 (confirmed animal carcinogen with unknown relevance to humans).

- ILO-WHO International Chemical Safety Cards (ICSCs)

10.7.5 Occupational Exposure Limits (OEL)

MAK (Maximale Arbeitsplatz Konzentration)

skin absorption (H); carcinogen category: 1; germ cell mutagen group: 3A

- ILO-WHO International Chemical Safety Cards (ICSCs)

10.7.6 Inhalation Risk

A harmful concentration of airborne particles can be reached quickly when dispersed.

- ILO-WHO International Chemical Safety Cards (ICSCs)

10.7.7 Effects of Short Term Exposure

The substance is irritating to the eyes and skin. The skin effects may appear after a latency period of a few hours.

- ILO-WHO International Chemical Safety Cards (ICSCs)

10.7.8 Effects of Long Term Exposure

This substance is carcinogenic to humans. May cause genetic damage in humans.

- ILO-WHO International Chemical Safety Cards (ICSCs)

10.7.9 Personal Protective Equipment (PPE)

Excerpt from NIOSH Pocket Guide for Propane sultone:

Skin: PREVENT SKIN CONTACT - Wear appropriate personal protective clothing to prevent skin contact.

Eyes: PREVENT EYE CONTACT - Wear appropriate eye protection to prevent eye contact.

Wash skin:

• WHEN CONTAMINATED - The worker should immediately wash the skin when it becomes contaminated.

• DAILY - The worker should wash daily at the end of each work shift, and prior to eating, drinking, smoking, etc.

Remove: WHEN WET OR CONTAMINATED - Work clothing that becomes wet or significantly contaminated should be removed and replaced.

Change: DAILY - Workers whose clothing may have become contaminated should change into uncontaminated clothing before leaving the work premises.

Provide:

• EYEWASH - Eyewash fountains should be provided in areas where there is any possibility that workers could be exposed to the substances; this is irrespective of the recommendation involving the wearing of eye protection.

• QUICK DRENCH - Facilities for quickly drenching the body should be provided within the immediate work area for emergency use where there is a possibility of exposure. [Note: It is intended that these facilities provide a sufficient quantity or flow of **water** to quickly remove the substance from any body areas likely to be exposed. The actual determination of what constitutes an adequate quick drench facility depends on the specific circumstances. In certain instances, a deluge shower should be readily available, whereas in others, the availability of **water** from a sink or hose could be considered adequate.] (NIOSH, 2024)

CAMEO Chemicals

PRECAUTIONS FOR "CARCINOGENS": ... Dispensers of liq detergent /should be available./ ... Safety pipettes should be used for all pipetting. ... In animal laboratory, personnel should ... wear protective suits (preferably disposable, one-piece & close-fitting at ankles & wrists), gloves, hair covering & overshoes. ... In chemical laboratory, gloves & gowns should always be worn ... however, gloves should not be assumed to provide full protection. Carefully fitted masks or respirators may be necessary when working with particulates or gases, & disposable plastic aprons might provide addnl protection. ... gowns ... /should be/ of distinctive color, this is a reminder that they are not to be worn outside the laboratory. /Chemical Carcinogens/

Montesano, R., H. Bartsch, E.Boyland, G. Della Porta, L. Fishbein, R. A. Griesemer, A.B. Swan, L. Tomatis, and W. Davis (eds.). Handling Chemical Carcinogens in the Laboratory: Problems of Safety. IARC Scientific Publications No. 33. Lyon, France: International Agency for Research on Cancer, 1979., p. 8

Hazardous Substances Data Bank (HSDB)

Wear appropriate personal protective clothing to prevent skin contact.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 265

- Hazardous Substances Data Bank (HSDB)

Wear appropriate eye protection to prevent eye contact.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 265

- Hazardous Substances Data Bank (HSDB)

Eyewash fountains should be provided in areas where there is any possibility that workers could be exposed to the substance; this is irrespective of the recommendation involving the wearing of eye protection.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 265

- Hazardous Substances Data Bank (HSDB)

For more Personal Protective Equipment (PPE) (Complete) data for 1,3-PROPANE SULTONE (7 total), please visit the HSDB record page.

- Hazardous Substances Data Bank (HSDB)

(See personal protection and sanitation codes)

Skin: Prevent skin contact - Wear appropriate personal protective clothing to prevent skin contact.

Eyes: Prevent eye contact - Wear appropriate eye protection to prevent eye contact.

Wash skin: When contaminated/Daily

Remove: When wet or contaminated

Change: Daily - Workers whose clothing may have become contaminated should change into uncontaminated clothing before leaving the work premises.

Provide: Eyewash, Quick drench

- The National Institute for Occupational Safety and Health (NIOSH)

10.7.10 Respirator Recommendations

NIOSH

At concentrations above the NIOSH REL, or where there is no REL, at any detectable concentration:

(APF = 10,000) Any self-contained breathing apparatus that has a full facepiece and is operated in a pressure-demand or other positive-pressure mode

(APF = 10,000) Any supplied-air respirator that has a full facepiece and is operated in a pressure-demand or other positive-pressure mode in combination with an auxiliary self-contained positive-pressure breathing apparatus

Escape:

(APF = 50) Any air-purifying, full-facepiece respirator (gas mask) with a chin-style, front- or back-mounted organic vapor canister having an N100, R100, or P100 filter.

Click here for information on selection of N, R, or P filters.

Any appropriate escape-type, self-contained breathing apparatus

Important additional information about respirator selection

- The National Institute for Occupational Safety and Health (NIOSH)

10.7.11 Preventions

Fire Prevention

NO open flames.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Exposure Prevention

See EFFECTS OF LONG-TERM OR REPEATED EXPOSURE. AVOID ALL CONTACT!

- ILO-WHO International Chemical Safety Cards (ICSCs)

Inhalation Prevention

Use closed system.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Skin Prevention

Protective gloves. Protective clothing.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Eye Prevention

Wear face shield or eye protection in combination with breathing protection.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Ingestion Prevention

Do not eat, drink, or smoke during work. Wash hands before eating.

- ILO-WHO International Chemical Safety Cards (ICSCs)

10.8 Stability and Reactivity

10.8.1 Air and Water Reactions

Soluble in water [Hawley].

- CAMEO Chemicals

10.8.2 Reactive Group

Acids, Strong Oxidizing

Sulfonates, Phosphonates, and Thiophosphonates, Organic

- CAMEO Chemicals

10.8.3 Reactivity Alerts

Water-Reactive

- CAMEO Chemicals

10.8.4 Reactivity Profile

PROPANE SULTONE reacts slowly with water to give 3-hydroxopropanesulfonic acid. This reaction may be accelerated by acid. May react with strong reducing agents to give toxic and flammable hydrogen sulfide.

- CAMEO Chemicals

10.8.5 Hazardous Reactivities and Incompatibilities

Evaporation of the residue after treatment of the thietane with hydrogen peroxide is liable to explode, and must be done in an open dish. This is probably because of formation of a 2 or 3-hydroperoxide derivative.

Bretherick, L. Handbook of Reactive Chemical Hazards. 2nd ed. Boston MA: Butterworths, 1979., p. 442

- **Hazardous Substances Data Bank (HSDB)**

10.9 Transport Information

10.9.1 Shipment Methods and Regulations

PRECAUTIONS FOR "CARCINOGENS": Procurement ... of unduly large amt ... should be avoided. To avoid spilling, carcinogens should be transported in securely sealed glass bottles or ampoules, which should themselves be placed inside strong screw-cap or snap-top container that will not open when dropped & will resist attack from the carcinogen. Both bottle & the outside container should be appropriately labelled. ... National post offices, railway companies, road haulage companies & airlines have regulations governing transport of hazardous materials. These authorities should be consulted before ... material is shipped. /Chemical Carcinogens/

Montesano, R., H. Bartsch, E.Boyland, G. Della Porta, L. Fishbein, R. A. Griesemer, A.B. Swan, L. Tomatis, and W. Davis (eds.). Handling Chemical Carcinogens in the Laboratory: Problems of Safety. IARC Scientific Publications No. 33. Lyon, France: International Agency for Research on Cancer, 1979., p. 13

- **Hazardous Substances Data Bank (HSDB)**

PRECAUTIONS FOR "CARCINOGENS": When no regulations exist, the following procedure must be adopted. The carcinogen should be enclosed in a securely sealed, watertight container (primary container), which should be enclosed in a second, unbreakable, leakproof container that will withstand chem attack from the carcinogen (secondary container). The space between primary & secondary container should be filled with absorbent material, which would withstand chem attack from the carcinogen & is sufficient to absorb the entire contents of the primary container in the event of breakage or leakage. Each secondary container should then be enclosed in a strong outer box. The space between the secondary container & the outer box should be filled with an appropriate quantity of shock-absorbent material. Sender should use fastest & most secure form of transport & notify recipient of its departure. If parcel is not received when expected, carrier should be informed so that immediate effort can be made to find it. Traffic schedules should be consulted to avoid ... arrival on weekend or holiday ... /Chemical Carcinogens/

Montesano, R., H. Bartsch, E.Boyland, G. Della Porta, L. Fishbein, R. A. Griesemer, A.B. Swan, L. Tomatis, and W. Davis (eds.). Handling Chemical Carcinogens in the Laboratory: Problems of Safety. IARC Scientific Publications No. 33. Lyon, France: International Agency for Research on Cancer, 1979., p. 13

- **Hazardous Substances Data Bank (HSDB)**

10.9.2 DOT Label

Poison

- CAMEO Chemicals

10.9.3 Packaging and Labelling

Do not transport with food and feedstuffs.

- ILO-WHO International Chemical Safety Cards (ICSCs)

10.9.4 EC Classification

Symbol: T; R: 45-21/22; S: 53-45; Note: E

- ILO-WHO International Chemical Safety Cards (ICSCs)

10.9.5 UN Classification

UN Hazard Class: 6.1; UN Pack Group: III

- ILO-WHO International Chemical Safety Cards (ICSCs)

10.10 Regulatory Information

The Australian Inventory of Industrial Chemicals

Chemical: 1,2-Oxathiolane, 2,2-dioxide

- Australian Industrial Chemicals Introduction Scheme (AICIS)

California Safe Cosmetics Program (CSCP) Reportable Ingredient

Hazard Traits - Carcinogenicity

Authoritative List - CA TACs; EC Annex VI CMRs - Cat. 1B; IARC Carcinogens - 2A; NTP RoC - reasonable; Prop 65

Report - regardless of intended function of ingredient in the product

- California Safe Cosmetics Program (CSCP) Product Database

REACH Registered Substance

Status: Active Update: 07-10-2022 https://echa.europa.eu/registration-dossier/-/registered-dossier/13407

Status: Active Update: 22-11-2012 https://echa.europa.eu/registration-dossier/-/registered-dossier/7444

- European Chemicals Agency (ECHA)

REACH Substances of Very High Concern (SVHC)

Substance: 1,3-propanesultone

EC: 214-317-9

Date of inclusion: >17-Dec-2015

Reason for inclusion: Carcinogenic (Article 57a)

https://echa.europa.eu/candidate-list-table

- European Chemicals Agency (ECHA)

New Zealand EPA Inventory of Chemical Status

1,3-Propane sultone: Does not have an individual approval but may be used under an appropriate group standard

- New Zealand Environmental Protection Authority (EPA)

10.10.1 Atmospheric Standards

Listed as a hazardous air pollutant (HAP) generally known or suspected to cause serious health problems. The Clean Air Act, as amended in 1990, directs EPA to set standards requiring major sources to sharply reduce routine emissions of toxic pollutants. EPA is required to establish and phase in specific performance based standards for all air emission sources that emit one or more of the listed pollutants. 1,3-Propane sultone is included on this list.

Clean Air Act as amended in 1990, Sect. 112 (b) (1) Public Law 101-549 Nov. 15, 1990

- Hazardous Substances Data Bank (HSDB)

10.10.2 CERCLA Reportable Quantities

Persons in charge of vessels or facilities are required to notify the National Response Center (NRC) immediately, when there is a release of this designated hazardous substance, in an amount equal to or greater than its reportable quantity of 10 lb or 4.54 kg. The toll free

number of the NRC is (800) 424-8802; In the Washington D.C. metropolitan area (202) 426-2675. The rule for determining when notification is required is stated in 40 CFR 302.4 (section IV. D.3.b).

54 FR 33419 (8/14/89)

- Hazardous Substances Data Bank (HSDB)

10.10.3 RCRA Requirements

As stipulated in 40 CFR 261.33, when 1,3-propane sultone, as a commercial chemical product or manufacturing chemical intermediate or an off-specification commercial chemical product or a manufacturing chemical intermediate, becomes a waste, it must be managed according to Federal and/or State hazardous waste regulations. Also defined as a hazardous waste is any residue, contaminated soil, water, or other debris resulting from the cleanup of a spill, into water or on dry land, of this waste. Generators of small quantities of this waste may qualify for partial exclusion from hazardous waste regulations (40 CFR 261.5).

40 CFR 261.33 (7/1/88)

- Hazardous Substances Data Bank (HSDB)

10.11 Other Safety Information

Chemical Assessment

IMAP assessments - 1,2-Oxathiolane, 2,2-dioxide: Human health tier II assessment

- Australian Industrial Chemicals Introduction Scheme (AICIS)

10.11.1 Toxic Combustion Products

When heated to decomposition propane sultone emits toxic fumes of SOx.

Sax, N.I. Dangerous Properties of Industrial Materials. 6th ed. New York, NY: Van Nostrand Reinhold, 1984., p. 2100

- Hazardous Substances Data Bank (HSDB)

10.11.2 Special Reports

National Toxicology Program. Eleventh Report on Carcinogens (2005). The Report on Carcinogens is an informational scientific and public health document that identifies and

discusses substances (including agents, mixtures, or exposure circumstances) that may pose a carcinogenic hazard to human health. 1,3-Propane Sultone (1120-71-4) is listed as reasonably anticipated to be a human carcinogen.[Available from, as of July 31, 2009: http://ntp.niehs.nih.gov/ntp/roc/eleventh/profiles/s153prop.pdf]

- Hazardous Substances Data Bank (HSDB)

11 Toxicity

11.1 Toxicological Information

11.1.1 NIOSH Toxicity Data

- The National Institute for Occupational Safety and Health (NIOSH)

11.1.2 Evidence for Carcinogenicity

The Human Health Assessment Group in EPA's Office of Health and Environmental Assessment has evaluated 1,3-Propane sultone for carcinogenicity. According to their analysis, the weight-of-evidence for 1,3-Propane sultone is group B2, which is based on no evidence in humans and sufficient evidence in animals. As a group B2 chemical, 1,3-Propane sultone is considered as probably carcinogenic to humans.

USEPA; Methodology for Evaluating Potential Carcinogenicity in Support of Reportable Quantity Adjustments Pursuant to Cercla Section 102 (Final) p. 42 (1988) EPA/600/8-89/053

- Hazardous Substances Data Bank (HSDB)

Evaluation: No epidemiological evidence relevant to the carcinogenicity of 1,3-propane sultone were available. There is sufficient evidence in experimental animals for the carcinogenicity of 1,3-propane sultone. Overall evaluation: 1,3-Propane sultone is possibly carcinogenic to humans (Group 2B).

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: ***https://monographs.iarc.fr/ENG/Classification/index.php****, p. V71 1101 (1999)*

- Hazardous Substances Data Bank (HSDB)

A3. Confirmed animal carcinogen with unknown relevance to humans.

American Conference of Governmental Industrial Hygienists TLVs and BEIs. Threshold Limit Values for Chemical Substances and Physical Agents and Biological Exposure Indices. Cincinnati, OH, 2008, p. 49

- Hazardous Substances Data Bank (HSDB)

1,3-Propane Sultone: reasonably anticipated to be a human carcinogen.

DHHS/National Toxicology Program; Eleventh Report on Carcinogens: 1,3-Propane Sultone (1120-71-4) (January 2005). Available from, as of July 31, 2009: ***https://ntp.niehs.nih.gov/ntp/roc/eleventh/profiles/s153prop.pdf***

- Hazardous Substances Data Bank (HSDB)

11.1.3 Carcinogen Classification

IARC Carcinogenic Agent	1,3-Propane sultone
IARC Carcinogenic Classes	Group 2A: Probably carcinogenic to humans
IARC Monographs	Volume 4: (1974) Some Aromatic Amines, Hydrazine and Related Substances, N-Nitroso Compounds and Miscellaneous Alkylating Agents Volume Sup 7: Overall Evaluations of Carcinogenicity: An Updating of IARC Monographs Volumes 1 to 42, 1987; 440 pages; ISBN 92-832-1411-0 (out of print) Volume 71: (1999) Re-evaluation of Some Organic Chemicals, Hydrazine and Hydrogen Peroxide (Part 1, Part 2, Part 3) Volume 110: (2017) Some Chemicals Used as Solvents and in Polymer Manufacture

Additional information	NB Overall evaluation upgraded to Group 2A with supporting evidence from other relevant data

- International Agency for Research on Cancer (IARC)

11.1.4 Exposure Routes

The substance can be absorbed into the body by inhalation, through the skin and by ingestion.

- ILO-WHO International Chemical Safety Cards (ICSCs)

inhalation, skin absorption, ingestion, skin and/or eye contact

- The National Institute for Occupational Safety and Health (NIOSH)

11.1.5 Symptoms

Skin Exposure

MAY BE ABSORBED! Redness. Pain. Burning sensation. Symptoms may be delayed.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Eye Exposure

Redness. Pain.

- ILO-WHO International Chemical Safety Cards (ICSCs)

irritation eyes, skin, respiratory system; [potential occupational carcinogen]

- The National Institute for Occupational Safety and Health (NIOSH)

11.1.6 Target Organs

Eyes, skin, respiratory system

- The National Institute for Occupational Safety and Health (NIOSH)

11.1.7 Cancer Sites

[in animals: skin tumors, leukemia, gliomas]

- The National Institute for Occupational Safety and Health (NIOSH)

11.1.8 Adverse Effects

IARC Carcinogen - Class 3: Chemicals are not classifiable by the International Agency for Research on Cancer.

NTP Carcinogen - Reasonably anticipated to be a human carcinogen.

ACGIH Carcinogen - Confirmed Animal.

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

11.1.9 Acute Effects

- ChemIDplus

11.1.10 Toxicity Data

LCLo (rat) = 2,140 mg/m3/6h

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

11.1.11 Interactions

1,3-PROPANE SULTONE-INDUCED SEEDLING GROWTH & ROOT GROWTH INJURY, M1 SPIKE STERILITY & M2 MUTATION FREQUENCY OF BARLEY INCR UNDER ACIDIC CONDITIONS OF PH IN **CITRATE PHOSPHATE** OR **PHTHALAN** SOLN.

SINGH C ET AL; INDIAN J EXP BIOL 17 (10): 1157 (1979)

- **Hazardous Substances Data Bank (HSDB)**

GROWTH REGULATORS **GIBBERELLIC ACID** AND **3-INDOLEACETIC ACID** EFFECTIVELY BLOCKED SEEDLING GROWTH INJURY AND MITOTIC CHROMOSOME ABERRATION INDUCTION BY THE ALKYLATING AGENT 1,3-PROPANE SULTONE IN BARLEY.

SINGH C & OLEJNICZAK J; GENET POL 20 (1): 43 (1979)

- **Hazardous Substances Data Bank (HSDB)**

SODIUM AZIDE-INDUCED MUTATION OF BARLEY WAS SIGNIFICANTLY ENHANCED BY PRIOR TREATMENT WITH 1,3-PROPANE SULTONE, WHEREAS NO SUCH INTERACTION WAS OBSERVED WHEN **SODIUM AZIDE**-PRETREATED SEEDS WERE EXPOSED TO 1,3-PROPANE SULTONE.

SINGH C ET AL; NUCLEUS (CALCUTTA) 23 (1-2): 63 (1980)

- **Hazardous Substances Data Bank (HSDB)**

The effects of 3 phenolic antioxidants, butylated hydroxyanisole, butylated hydroxytoluene, and **propyl gallate** on the mutagenic activity of propane sultone were studied using barley (Hordeum vulgare) as the test system. The antioxidants produced seedling injury marginally but did not produce any chromosomal aberrations. When administered either prior to propane sultone treatment or in a mixture with it, the seedling injury, chromosomal aberrations, mutation per 100 ml spikes as well as M2 chlorophyll mutation frequency, were enhanced. Post treatments reduced M1 spike sterility, mutations per 100 ml spikes and M2 chlorophyll mutation frequency.

PMID:7242545

Kaul B, Tandor V; Mutat Res 89 (1): 57-62 (1981)

- **Hazardous Substances Data Bank (HSDB)**

In Chinese hamster (K1) cells and human lymphocytes treated with anticancer antibiotics and propane sultone, hyperthermia increased the potential of these compounds to induce chromosome aberrations when applied at temperature higher than 37 °C, irrespective of cell cycle phase.

Vig BK et al; Cytogenet Cell Gen 33 (1-2): 35-41 (1982)

- Hazardous Substances Data Bank (HSDB)

11.1.12 Medical Surveillance

PRECAUTIONS FOR "CARCINOGENS": Whenever medical surveillance is indicated, in particular when exposure to a carcinogen has occurred, ad hoc decisions should be taken concerning ... /cytogenetic and/or other/ tests that might become useful or mandatory. /Chemical Carcinogens/

Montesano, R., H. Bartsch, E.Boyland, G. Della Porta, L. Fishbein, R. A. Griesemer, A.B. Swan, L. Tomatis, and W. Davis (eds.). Handling Chemical Carcinogens in the Laboratory: Problems of Safety. IARC Scientific Publications No. 33. Lyon, France: International Agency for Research on Cancer, 1979., p. 23

- Hazardous Substances Data Bank (HSDB)

11.1.13 Human Toxicity Excerpts

INDUCTION OF ANCHORAGE-INDEPENDENT GROWTH IN HUMAN FIBROBLASTS BY PROPANE SULTONE.

PMID:7214333

SILINSKAS KC ET AL; CANCER RES 41 (5): 1620 (1981)

- Hazardous Substances Data Bank (HSDB)

. HUMAN FORESKIN EPITHELIAL CELLS WERE TRANSFORMED TO AN ANCHORAGE-INDEPENDENT STATE OF GROWTH (IN SOFT AGAR) AND NEOPLASIA (INVASION OF CHICK EMBRYONIC SKIN IN VITRO).

PMID:6171346

MILO GE ET AL; CANCER RES 41 (12, PART 1): 5096 (1981)

- Hazardous Substances Data Bank (HSDB)

Genotoxicological investgation of 1,3-propane sultone was undertaken using human lymphocyte cultures as the test system. Concentrations greater than 1mM induced appreciable chromosomal aberrations, which increased proportionally to the dose or the duration of treatment. It was lso observed that treatment administred t 45 degrees C produced almost 3 times more abnormal cells than at 37 degrees C. The chemical also produced a significantly higher frequency of sister chromatid exchanges.

PMID:4071562

Kaul BL; Toxicol Lett 28 (2-3): 139-42 (1985)

- Hazardous Substances Data Bank (HSDB)

11.1.14 Non-Human Toxicity Excerpts

IN 3/8 /BD/ RATS SURVIVING 381-492 DAYS AFTER WEEKLY /IV/ INJECTIONS OF 20 MG/KG BODY WT /DEVELOPED/ ... 1 NEPHROBLASTOMA, 1 CARCINOMA OF ILEOCECAL REGION & 1 MIXED GLIAL-MESODERMAL TUMOR OF BRAIN TOGETHER WITH A MAMMARY CARCINOMA ... .

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 256 (1974)*

- Hazardous Substances Data Bank (HSDB)

IN 2/12 /BD/ RATS GIVEN 10 MG/KG BODY WT/WK /IV/ ... 1 GANGLIONEUROMA OF ADRENAL GLAND & 1 NEUROCYTOMA OF TRIGEMINUS NERVE DEVELOPED AFTER 296 & 469 DAYS. OF 32 RATS GIVEN SINGLE DOSE OF 150 MG/KG BODY WT, 1 DIED AFTER 235 DAYS WITH GLIOMA OF BRAIN, & 9 DIED WITH MALIGNANT TUMORS @ VARIETY OF SITES WITHIN 459 DAYS.

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 256 (1974)*

- Hazardous Substances Data Bank (HSDB)

SINGLE IV INJECTION OF 20 MG/KG BODY WT ... GIVEN TO PREGNANT RATS ON 15TH DAY OF GESTATION PRODUCED MALIGNANT NEUROGENIC TUMORS IN 3/25 OFFSPRING; DOSE OF 60 MG/KG BODY WT PRODUCED MALIGNANT TUMORS IN 4/14 OFFSPRING, INCLUDING 2 NEUROGENIC TUMORS, 1 TUMOR OF PANCREAS & 1 OF OVARY.

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 257 (1974)*

- Hazardous Substances Data Bank (HSDB)

WEEKLY /IV/ INJECTIONS OF 2% SOLN ... IN **WATER** TO 10 BD RATS @ ... 40 MG/KG ... TREATMENT WAS STOPPED AFTER 16 WK (TOTAL DOSE, 560 MG/KG BODY WT) ... IN 1 RAT ... SARCOMA OF MEDIASTINUM WITH METASTASES IN RIGHT LUNG & KIDNEY ... OBSERVED. IN 2 RATS ... 1 GLIAL-MESODERMAL MIXED TUMOR OF BRAIN & 1 NEUROSARCOMA OF PLEXUS CERVICALIS ... .

IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work).

*Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 256 (1974)*

- **Hazardous Substances Data Bank (HSDB)**

For more Non-Human Toxicity Excerpts (Complete) data for 1,3-PROPANE SULTONE (15 total), please visit the **HSDB record page**.

- **Hazardous Substances Data Bank (HSDB)**

11.1.15 Non-Human Toxicity Values

TD Rat oral: 12 g/kg/ 60 wk continuous.

NIOSH; Current Awareness Listing (1984)

- **Hazardous Substances Data Bank (HSDB)**

TD Rat oral: 13 g/kg/32 wk continuous.

NIOSH; Current Awareness Listing (1984)

- **Hazardous Substances Data Bank (HSDB)**

TD Rat subcutaneous: 166 mg/kg

NIOSH; Current Awareness Listing (1984)

- **Hazardous Substances Data Bank (HSDB)**

TD Rat subcutaneous: 559 mg/kg/17 wk intermittent

NIOSH; Current Awareness Listing (1984)

- **Hazardous Substances Data Bank (HSDB)**

For more Non-Human Toxicity Values (Complete) data for 1,3-PROPANE SULTONE (9 total), please visit the **HSDB record page**.

- **Hazardous Substances Data Bank (HSDB)**

11.2 Ecological Information

11.2.1 ICSC Environmental Data

Environmental effects from the substance have not been investigated adequately.

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.2.2 Environmental Fate / Exposure Summary

1,3-Propane sultone may be released to the environment as a result of its manufacture and use as a chemical intermediate. If 1,3-propane sultone is released to soil, it will be expected to rapidly hydrolyze if the soil is moist, based upon the rapid hydrolysis observed in aqueous solution. Since it rapidly hydrolyzes, adsorption to and volatilization from moist soil are not expected to be significant processes, although no data specifically regarding the fate of 1,3-propane sultone in soil were located. If released to **water**, it will be expected to rapidly hydrolyze, based upon a measured rate constant of 8.2X10-2 hr-1 for hydrolysis in aqueous solution at 25 °C which corresponds to a half-life of 8.5 hr. The product of hydrolysis is 3-hydroxy-1-propanesulphonic acid. Since it rapidly hydrolyzes, bioconcentration, volatilization, and adsorption to sediment and suspended solids are not expected to be significant processes. No data were located concerning biodegradation, but 1,3-propane sultone will probably abiotically hydrolyze significantly faster than it biodegrades. If released to the atmosphere, it will be susceptible to photooxidation via vapor phase reaction with photochemically produced hydroxyl radicals with a half-life of 8 days estimated for this process. Exposure to 1,3-propane sultone will be primarily occupational. (SRC)

- Hazardous Substances Data Bank (HSDB)

11.2.3 Natural Pollution Sources

There are no known natural sources of 1,3-propane sultone(1).

(1) IARC; Monograph on the Evaluation of the Carcinogenic Risk of Chemicals to Humans 4: 253-5 (1974)

- Hazardous Substances Data Bank (HSDB)

11.2.4 Artificial Pollution Sources

ENVIRONMENTAL PERSISTENCE: IT MAY OCCUR IN WASTE STREAMS OF PLANTS MAKING OR USING IT, BUT BECAUSE IT IS READILY HYDROLYZED IT WOULD NOT BE EXPECTED TO REMAIN AS SUCH FOR PROTRACTED PERIODS OF TIME.

*IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work). Available at: **https://monographs.iarc.fr/ENG/Classification/index.php**, p. V4 255 (1974)*

- Hazardous Substances Data Bank (HSDB)

1,3-Propane sultone may be released to the environment as a result of its manufacture and use as an intermediate in the production of a large number of sulfopropylated products possibly including detergents, wetting agents, surfactants, dyes, soluble starches, cation-exchange resins, and insecticides(1).

(1) IARC; Monograph on the Evaluation of the Carcinogenic Risk of Chemicals to Humans 4: 253-5 (1974)

Hazardous Substances Data Bank (HSDB)

11.2.5 Environmental Fate

TERRESTRIAL FATE: If 1,3-propane sultone is released to soil, it will be expected to rapidly hydrolyze if the soil is moist, based upon the rapid hydrolysis observed in aqueous solution(1,2,SRC). Since it rapidly hydrolyzes, adsorption to and volatilization from moist soil are not expected to be significant processes, although no data specifically regarding the fate of 1,3-propane sultone in soil were located(SRC).

(1) Ellington JJ et al; Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal: Vol 3 USEPA-600/3-88/028 (NTIS PB88-23042/AS)

(2) Bordwell FG et al; J Am Chem Soc 81: 2698-705 (1958)

Hazardous Substances Data Bank (HSDB)

AQUATIC FATE: If 1,3-propane sultone is released to **water**, it will be expected to rapidly hydrolyze, based upon a measured rate constant of 8.2X10-2 hr-1 for hydrolysis in aqueous solution at 25 °C(1) which corresponds to a half-life of 8.5 hr(SRC). The product of hydrolysis is 3-hydroxy-1-propanesulphonic acid(2). Since it rapidly hydrolyzes, bioconcentration, volatilization, and adsorption to sediment and suspended solids are not expected to be significant processes((SRC). No data were located concerning biodegradation, but 1,3-propane sultone will probably abiotically hydrolyze significantly faster than biodegradation(SRC).

(1) Ellington JJ et al; Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal Vol 3 USEPA-600/3-88/028 (NTIS PB88-23042/AS)

(2) IARC; Monograph on the Evaluation of the Carcinogenic Risk of Chemicals to Humans 4: 253-5 (1974)

Hazardous Substances Data Bank (HSDB)

ATMOSPHERIC FATE: If 1,3-propane sultone is released to the atmosphere, it will be susceptible to photooxidation via vapor phase reaction with photochemically produced hydroxyl radicals. An atmospheric half-life of 8 days at an atmospheric concentration of 5X10+5 hydroxyl radicals per cu cm has been calculated for this process based upon an estimated rate constant(1,SRC).

(1) Atkinson R; Intern J Chem Kinetics 19: 799-828 (1987)

- Hazardous Substances Data Bank (HSDB)

11.2.6 Environmental Biodegradation

No data were located concerning the biodegradation of 1,3-propane sultone either in natural systems or in laboratory studies(SRC). Since 1,3-propane sultone rapidly hydrolyzes in **water** (1,2), biodegradation probably will not be a significant process in the environment(SRC).

(1) Ellington JJ et al; Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal Vol 3 USEPA-600/3-88/028 (NTIS PB88-23042/AS)

(2) Bordwell FG et al; J Am Chem Soc 81: 2698-705 (1958)

- Hazardous Substances Data Bank (HSDB)

11.2.7 Environmental Abiotic Degradation

A measured overall rate constant for hydrolysis of 1,3-propane sultone in aqueous solution at 25 °C of 8.2X10-2 hr-1 has been reported(1). This corresponds to a half-life of 8.5 hr at 25 °C(1,SRC). Another reported overall rate constant for hydrolysis is 1X10-6 sec-1 at 20 °C(3), which corresponds to a half-life of 8 days(3,SRC). The hydrolysis has been reported to be base-catalyzed(4) suggesting that hydrolysis may be faster in alkaline waters and slower in acidic waters relative to the rate of hydrolysis in neutral solution(SRC). The product of hydrolysis is 3-hydroxy-1-propanesulphonic acid(5). The rate of hydrolysis in air has been estimated to be negligibly slow(4). The rate constant for the vapor phase reaction of 1,3-propane sultone with photochemically produced hydroxyl radicals has been estimated to be 2X10-12 cu cm/molecule-sec at 25 °C which corresponds to an atmospheric half-life of 8 days at an atmospheric concentration of 5X10+5 hydroxyl radicals per cu cm(2,SRC).

(1) Ellington JJ et al; Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal Vol 3 USEPA-600/3-88/028 (NTIS PB88-23042/AS) (1988)

(2) Atkinson R; Intern J Chem Kinetics 19: 799-828 (1987)

(3) Bordwell FG et al; J Am Chem Soc 81: 2698-705 (1958)

(4) Radding SB et al; Review of the environmental fate of selected chemicals (NTIS 68-01-2681) (1977)

(5) IARC; Monograph on the Evaluation of the Carcinogenic Risk of Chemicals to Humans 4: 253-5 (1974)

- Hazardous Substances Data Bank (HSDB)

11.2.8 Environmental Bioconcentration

Since 1,3-propane sultone hydrolyzes rapidly in water(1,2), bioconcentration in aquatic organisms is not expected to be a significant process(SRC).

(1) Ellington JJ et al; Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal Vol 3 USEPA-600/3-88/028 (NTIS PB88-23042/AS)

(2) Bordwell FG et al; J Am Chem Soc 81: 2698-705 (1958)

- **Hazardous Substances Data Bank (HSDB)**

11.2.9 Soil Adsorption / Mobility

Since 1,3-propane sultone hydrolyzes rapidly in water(1,2), and presumably in moist soil(SRC), adsorption to soil is not expected to be a significant process(SRC).

(1) Ellington JJ et al; Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal Vol 3 USEPA-600/3-88/028 (NTIS PB88-23042/AS)

(2) Bordwell FG et al; J Am Chem Soc 81: 2698-705 (1958)

- **Hazardous Substances Data Bank (HSDB)**

11.2.10 Volatilization from Water / Soil

Due to a lack of data, it is not possible to estimate the half-life for volatilization from water or soil(SRC). Volatilization of 1,3-propane sultone from water and moist soil, however, is not expected to be significant since the compound hydrolyzes rapidly in water(1,2,SRC).

(1) Ellington JJ et al; Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal Vol 3 USEPA-600/3-88/028 (NTIS PB88-23042/AS)

(2) Bordwell FG et al; J Am Chem Soc 81: 2698-705 (1958)

- **Hazardous Substances Data Bank (HSDB)**

11.2.11 Probable Routes of Human Exposure

Exposure to 1,3-propane sultone will be primarily occupational, but the routes of exposure are difficult to evaluate due to a lack of data. (SRC)

- **Hazardous Substances Data Bank (HSDB)**

12 Associated Disorders and Diseases

Comparative Toxicogenomics Database (CTD)

13 Literature

13.1 Consolidated References

PubChem

13.2 NLM Curated PubMed Citations

PubChem

13.3 Springer Nature References

Springer Nature

13.4 Thieme References

Thieme Chemistry

13.5 Wiley References

Wiley

13.6 Nature Journal References

Ma et al. Acyclic cucurbit[n]uril molecular containers enhance the solubility and bioactivity of poorly soluble pharmaceuticals. Nature Chemistry, doi: 10.1038/nchem.1326, published online 15 April 2012 http://www.nature.com/nchem

Nature Chemistry

13.7 Chemical Co-Occurrences in Literature

PubChem

13.8 Chemical-Gene Co-Occurrences in Literature

PubChem

13.9 Chemical-Disease Co-Occurrences in Literature

PubChem

14 Patents

14.1 Depositor-Supplied Patent Identifiers

PubChem

Link to all deposited patent identifiers

PubChem

14.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=FSSPGSAQUIYDCN-UHFFFAOYSA-N

- PATENTSCOPE (WIPO)

14.3 Chemical Co-Occurrences in Patents

- PubChem

14.4 Chemical-Disease Co-Occurrences in Patents

PubChem

14.5 Chemical-Gene Co-Occurrences in Patents

PubChem

15 Interactions and Pathways

15.1 Chemical-Target Interactions

Comparative Toxicogenomics Database (CTD)

16 Biological Test Results

16.1 BioAssay Results

PubChem

17 Classification

17.1 MeSH Tree

Medical Subject Headings (MeSH)

17.2 ChEBI Ontology

ChEBI

17.3 ChemIDplus

ChemIDplus

17.4 CAMEO Chemicals

CAMEO Chemicals

17.5 UN GHS Classification

GHS Classification (UNECE)

17.6 NORMAN Suspect List Exchange Classification

NORMAN Suspect List Exchange

17.7 EPA DSSTox Classification

EPA DSSTox

17.8 International Agency for Research on Cancer (IARC) Classification

International Agency for Research on Cancer (IARC)

17.9 EPA TSCA and CDR Classification

EPA Chemicals under the TSCA

17.10 EPA Substance Registry Services Tree

EPA Substance Registry Services

18 Information Sources

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1. **Australian Industrial Chemicals Introduction Scheme (AICIS)**

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   1,2-Oxathiolane, 2,2-dioxide
   https://services.industrialchemicals.gov.au/search-assessments/

   1,2-Oxathiolane, 2,2-dioxide
   https://services.industrialchemicals.gov.au/search-inventory/

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   PROPANE SULTONE
   https://cameochemicals.noaa.gov/chemical/16123

   CAMEO Chemical Reactivity Classification
   https://cameochemicals.noaa.gov/browse/react

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   Propane sultone
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4. **ChemIDplus**

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1,3-Propane sultone

https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0001120714

ChemIDplus Chemical Information Classification

https://pubchem.ncbi.nlm.nih.gov/source/ChemIDplus

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Propane sultone

https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=42386

6. EPA Chemicals under the TSCA

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https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

1,2-Oxathiolane, 2,2-dioxide

https://www.epa.gov/chemicals-under-tsca

EPA TSCA Classification

https://www.epa.gov/tsca-inventory

7. EPA DSSTox

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https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

1,3-Propane sultone

https://comptox.epa.gov/dashboard/DTXSID8021195

CompTox Chemicals Dashboard Chemical Lists

https://comptox.epa.gov/dashboard/chemical-lists/

8. European Chemicals Agency (ECHA)

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https://echa.europa.eu/web/guest/legal-notice

1,3-propanesultone

https://chem.echa.europa.eu/100.013.017

1,3-propanesultone (EC: 214-317-9)

https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/131254

9. FDA Global Substance Registration System (GSRS)

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https://www.fda.gov/about-fda/about-website/website-policies#linking

1,3-PROPANE SULTONE

https://gsrs.ncats.nih.gov/ginas/app/beta/substances/L6NTK7VJX9

10. Hazardous Substances Data Bank (HSDB)

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https://www.nlm.nih.gov/web_policies.html

1,3-PROPANE SULTONE

https://pubchem.ncbi.nlm.nih.gov/source/hsdb/1673

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1,3-PROPANE SULTONE

https://www.ilo.org/dyn/icsc/showcard.display?p_version=2&p_card_id=1524

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1,3-Propane sultone

https://www.epa.govt.nz/industry-areas/hazardous-substances/guidance-for-importers-and-manufacturers/hazardous-substances-databases/

13. The National Institute for Occupational Safety and Health (NIOSH)

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1,2-Oxathiolane 2,2-dioxide

https://www.cdc.gov/niosh-rtecs/RP52C768.html

Propane sultone

https://www.cdc.gov/niosh/npg/npgd0525.html

14. ## California Safe Cosmetics Program (CSCP) Product Database

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https://www.cdph.ca.gov/Pages/Conditions-of-Use.aspx

1,3-Propane sultone

https://www.cdph.ca.gov/Programs/CCDPHP/DEODC/OHB/CSCP/Pages/About-CSCP.aspx

15. ## California Office of Environmental Health Hazard Assessment (OEHHA)

1,3-Propane Sultone

https://oehha.ca.gov/proposition-65/chemicals/13-propane-sultone

16. ## ChEBI

1,3-Propane sultone

https://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:82370

ChEBI Ontology

http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology

17. ## EPA Air Toxics

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https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

1,3-Propane Sultone

https://www.epa.gov/sites/default/files/2016-09/documents/1-3-propane-sultone.pdf

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https://ncithesaurus.nci.nih.gov/ncitbrowser/ConceptReport.jsp?dictionary=NCI_Thesaurus&ns=ncit&code=C44437

19. ## NJDOH RTK Hazardous Substance List

1,2-oxathiolane 2,2-dioxide

http://nj.gov/health/eoh/rtkweb/documents/fs/1446.pdf

20. ## Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

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https://haz-map.com/About

Propane sultone

https://haz-map.com/Agents/420

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http://www.ebi.ac.uk/Information/termsofuse.html

https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL3185243/

22. Comparative Toxicogenomics Database (CTD)

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http://ctdbase.org/about/legal.jsp

1,3-propane sultone

https://ctdbase.org/detail.go?type=chem&acc=C003218

23. Crystallography Open Database (COD)

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24. Hazardous Chemical Information System (HCIS), Safe Work Australia

1,3-propanesultone

http://hcis.safeworkaustralia.gov.au/HazardousChemical/Details?chemicalID=3663

25. NITE-CMC

1,2-Oxathiolane 2,2-dioxide - FY2010 (Revised classification)

https://www.nite.go.jp/chem/english/ghs/10-mhlw-2028e.html

1,2-Oxathiolane 2,2-dioxide - FY2006 (New/original classication)

https://www.nite.go.jp/chem/english/ghs/06-imcg-0234e.html

1,2-Oxathiolane 2,2-dioxide; 1,3-Propane sultone - FY2020 (Revised classification)

https://www.nite.go.jp/chem/english/ghs/20-mhlw-2085e.html

26. Regulation (EC) No 1272/2008 of the European Parliament and of the Council

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1,3-propanesultone; 1,2-oxathiolane 2,2-dioxide

https://eur-lex.europa.eu/eli/reg/2008/1272/2023-07-31

27. Human Metabolome Database (HMDB)

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1,3-Propane sultone

http://www.hmdb.ca/metabolites/HMDB0244180

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1,3-Propane sultone

https://monographs.iarc.who.int/list-of-classifications

IARC Classification

https://www.iarc.fr/

29. Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J4.528D

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J778.863K

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https://www.kegg.jp/entry/C19296

31. Nature Chemistry

https://pubchem.ncbi.nlm.nih.gov/substance/135363110

32. NIST Mass Spectrometry Data Center

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Data covered by the Standard Reference Data Act of 1968 as amended.
https://www.nist.gov/srd/public-law

1,2-Oxathiolane, 2,2-dioxide

http://www.nist.gov/srd/nist1a.cfm

33. ## SpectraBase

1,2-OXATHIOLANE, 2,2-DIOXIDE
https://spectrabase.com/spectrum/Iy36W9zX487

1,2-Oxathiolane, 2,2-dioxide
https://spectrabase.com/spectrum/8OdW3xEMdj6

1,2-OXATHIOLANE, 2,2-DIOXIDE
https://spectrabase.com/spectrum/3b3x9x70tBf

1,2-Oxathiolane-2,2-dioxide
https://spectrabase.com/spectrum/FgfXpnFxqXb

1,2-oxathiolane, 2,2-dioxide
https://spectrabase.com/spectrum/62S4QR8cqcN

1,3-Propanesultone
https://spectrabase.com/spectrum/5hNhDRqCcdp

1,2-OXATHIOLANE, 2,2-DIOXIDE
https://spectrabase.com/spectrum/LpopAGMimWp

1,2-OXATHIOLANE, 2,2-DIOXIDE
https://spectrabase.com/spectrum/5bvRBF3PNRZ

1,2-OXATHIOLANE, 2,2-DIOXIDE
https://spectrabase.com/spectrum/4rPO31wSfPs

1,3-Propane sultone
https://spectrabase.com/spectrum/HVaGoBJV28E

1,3-Propanesultone
https://spectrabase.com/spectrum/4r2D0oBdYha

34. ## Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=7047337-192438107

35. ## SpringerMaterials

3-hydroxy-1-propanesulfonic acid w-sultone
https://materials.springer.com/substanceprofile/docs/smsid_hyjqrvcbixcripve

36. ## The Cambridge Structural Database

https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=139566

37. ## Thieme Chemistry

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https://creativecommons.org/licenses/by-nc-nd/4.0/

https://pubchem.ncbi.nlm.nih.gov/substance/?source=22163&sourceid=7047337-192438107

38. ## Wikidata

LICENSE
CCZero
https://creativecommons.org/publicdomain/zero/1.0/

1,3-propane sultone
https://www.wikidata.org/wiki/Q1933902

39. ## Wikipedia

Alfetamine
https://en.wikipedia.org/wiki/Alfetamine

1,3-Propane sultone
https://en.wikipedia.org/wiki/1,3-Propane_sultone

40. ## Wiley

https://pubchem.ncbi.nlm.nih.gov/substance/?source=wiley&sourceid=181239

41. PubChem

https://pubchem.ncbi.nlm.nih.gov

42. ## Medical Subject Headings (MeSH)

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https://www.nlm.nih.gov/copyright.html

1,3-propane sultone
https://www.ncbi.nlm.nih.gov/mesh/67003218

MeSH Tree
http://www.nlm.nih.gov/mesh/meshhome.html

43. ## GHS Classification (UNECE)

GHS Classification Tree
http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

44. ## NORMAN Suspect List Exchange

LICENSE
Data: CC-BY 4.0; Code (hosted by ECI, LCSB): Artistic-2.0
https://creativecommons.org/licenses/by/4.0/

NORMAN Suspect List Exchange Classification
https://www.norman-network.com/nds/SLE/

45. ## EPA Substance Registry Services

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

EPA SRS List Classification
https://sor.epa.gov/sor_internet/registry/substreg/LandingPage.do

46. **PATENTSCOPE (WIPO)**

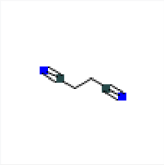
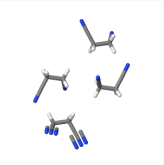
SID 403391104
https://pubchem.ncbi.nlm.nih.gov/substance/403391104

47. NCBI

https://www.ncbi.nlm.nih.gov/projects/linkout

COMPOUND SUMMARY

Succinonitrile

PubChem CID	8062
Structure	 2D 3D  Crystal
Chemical Safety	Acute Toxic Irritant Environmental Hazard Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_4H_4N_2$ $CNCH_2CH_2CN$
Synonyms	SUCCINONITRILE Butanedinitrile 110-61-2 1,2-Dicyanoethane Deprelin View More...
Molecular Weight	80.09 g/mol *Computed by PubChem 2.2 (PubChem release 2021.10.14)*
Dates	Create: 2005-03-26 Modify: 2024-10-26
Description	Succinonitrile appears as colorless to light brown crystals. Colorless waxy solid melting at 57 °C. Highly toxic.

- CAMEO Chemicals

Succinonitrile is a chemical compound of cyanide.

- Toxin and Toxin Target Database (T3DB)

Contents

Title and Summary

1 Structures

2 Names and Identifiers

3 Chemical and Physical Properties

4 Spectral Information

5 Related Records

6 Chemical Vendors

7 Drug and Medication Information

8 Pharmacology and Biochemistry

9 Use and Manufacturing

10 Identification

11 Safety and Hazards

12 Toxicity

13 Literature

14 Patents

15 Interactions and Pathways

16 Biological Test Results

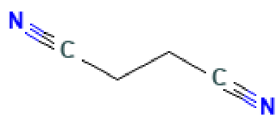
17 Classification

18 Information Sources

1 Structures

1.1 2D Structure

Chemical Structure Depiction

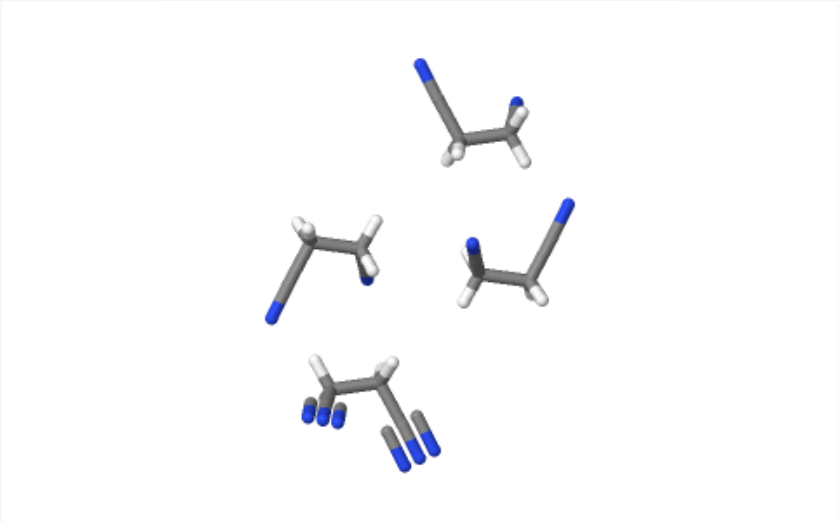


PubChem

1.2 3D Conformer

PubChem

1.3 Crystal Structures

1 of 4	View All
CCDC Number	702139
Associated Article	DOI:10.1002/zaac.200800404
Crystal Structure Data	DOI:10.5517/ccrkmnk
Crystal Structure Depiction	

The Cambridge Structural Database

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

butanedinitrile

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

PubChem

2.1.2 InChI

InChI=1S/C4H4N2/c5-3-1-2-4-6/h1-2H2

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

- PubChem

2.1.3 InChIKey

IAHFWCOBPZCAEA-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

- PubChem

2.1.4 SMILES

C(CC#N)C#N

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

- PubChem

2.2 Molecular Formula

$C_4H_4N_2$

Computed by PubChem 2.2 (PubChem release 2021.10.14)

- Australian Industrial Chemicals Introduction Scheme (AICIS); CAMEO Chemicals; PubChem

$C_4H_4N_2$

$CNCH_2CH_2CN$

- ILO-WHO International Chemical Safety Cards (ICSCs)

2.3 Other Identifiers

2.3.1 CAS

110-61-2

- Australian Industrial Chemicals Introduction Scheme (AICIS); CAMEO Chemicals; CAS Common C...

2.3.2 Deprecated CAS

191362-21-7

- ChemIDplus; EPA Chemicals under the TSCA

2.3.3 European Community (EC) Number

203-783-9

- European Chemicals Agency (ECHA)

2.3.4 UNII

1R479O92DO

- FDA Global Substance Registration System (GSRS)

2.3.5 UN Number

3276

- ILO-WHO International Chemical Safety Cards (ICSCs)

2.3.6 ChEMBL ID

CHEMBL1562258

- ChEMBL

2.3.7 DSSTox Substance ID

DTXSID9026059

- EPA DSSTox

2.3.8 HMDB ID

HMDB0258544

- Human Metabolome Database (HMDB)

2.3.9 ICSC Number

1497

- ILO-WHO International Chemical Safety Cards (ICSCs)

2.3.10 Nikkaji Number

J2.450C

- Japan Chemical Substance Dictionary (Nikkaji)

2.3.11 NSC Number

4852

- DTP/NCI

2.3.12 RTECS Number

WN3850000

- The National Institute for Occupational Safety and Health (NIOSH)

2.3.13 Wikidata

Q3502773

- Wikidata

2.3.14 Wikipedia

M-Cresol

- Wikipedia

Succinonitrile

- Wikipedia

2.4 Synonyms

2.4.1 MeSH Entry Terms

succinonitrile

- Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

SUCCINONITRILE	Ethylene dicyanide	Ethane, 1,2-dicyano-	BRN 1098380	EC 20
Butanedinitrile	Succinil	USAF A-9442	DTXSID9026059	Sukci
110-61-2	Disuxyl	Sukcinonitril [Czech]	AI3-06591	sDicy
1,2-Dicyanoethane	Evanex	sym-Dicyanoethane	1R479O92DO	1,2Di
Deprelin	Suxil	1,2-dicyano-ethan	NCCH2CH2CN	1,4Bu
Succinodinitrile	s-Dicyanoethane	NSC 4852	NSC-4852	Ethar
Ethylene cyanide	Succinic dinitrile	CCRIS 4720	SUCCINONITRILE [MI]	MFCD
Dician	Succinic acid nitrile	HSDB 7190	SUCCINONITRILE [HSDB]	Ethar
Dinile	Succinic acid dinitrile	EINECS 203-783-9	DTXCID706059	Succi
1,4-Butanedinitrile	Sukcinonitril	UNII-1R479O92DO	SUCCINONITRILE [WHO-DD]	1, 4-B

- PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference

Molecular Weight	80.09 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
XLogP3	-1	Computed by XLogP3 3.0 (PubChem release 2021.10.14)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Hydrogen Bond Acceptor Count	2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Rotatable Bond Count	1	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Exact Mass	80.037448136 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Monoisotopic Mass	80.037448136 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Topological Polar Surface Area	47.6$Å^2$	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Heavy Atom Count	6	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	92	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.10.14)

- PubChem

3.2 Experimental Properties

3.2.1 Physical Description

Succinonitrile appears as colorless to light brown crystals. Colorless waxy solid melting at 57 °C. Highly toxic.

- CAMEO Chemicals

Colorless, odorless, waxy solid; Note: Forms cyanide in the body; [NIOSH]

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

COLOURLESS WAXY CRYSTALS.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Colorless, odorless, waxy solid. [Note: Forms cyanide in the body.]

- The National Institute for Occupational Safety and Health (NIOSH)

3.2.2 Color / Form

Colorless waxy solid

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 467

- Hazardous Substances Data Bank (HSDB)

3.2.3 Odor

Odorless

NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases. U.S. Department of Health & Human Services, Public Health Service, Center for Disease Control & Prevention. DHHS (NIOSH) Publication No. 2001-145 (CD-ROM) August 2001.

- Hazardous Substances Data Bank (HSDB)

3.2.4 Boiling Point

509 to 513 °F at 760 mmHg (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

- **CAMEO Chemicals**

266 °C

Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 81st Edition. CRC Press LLC, Boca Raton: FL 2000, p. 3-92

- **Hazardous Substances Data Bank (HSDB)**

Boiling point: 185 °C @ 60 mm Hg; 158-160 @ 20 mm Hg

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 1580

- **Hazardous Substances Data Bank (HSDB)**

265 °C

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

509 °F

- **The National Institute for Occupational Safety and Health (NIOSH)**

3.2.5 Melting Point

135 to 136 °F (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

- **CAMEO Chemicals**

54.5 °C

Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 81st Edition. CRC Press LLC, Boca Raton: FL 2000, p. 3-92

- Hazardous Substances Data Bank (HSDB)

54 °C

- ILO-WHO International Chemical Safety Cards (ICSCs)

134 °F

- The National Institute for Occupational Safety and Health (NIOSH)

3.2.6 Flash Point

270 °F (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

- CAMEO Chemicals

132 °C

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases; ILO-WHO Internation…

270 °F (132 °C) (closed cup)

Fire Protection Guide to Hazardous Materials. 13 ed. Quincy, MA: National Fire Protection Association, 2002., p. 325-104

- Hazardous Substances Data Bank (HSDB)

270 °F

- The National Institute for Occupational Safety and Health (NIOSH)

3.2.7 Solubility

50 to 100 mg/mL at 70 °F (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

- CAMEO Chemicals

Soluble in acetone, chloroform, dioxane; slightly soluble in ethanol, benzene, ether, carbon sulfide

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 1580

- **Hazardous Substances Data Bank (HSDB)**

In water, 126.9 g/L @ 20 °C

Yalkowsky, S.H., He, Yan., Handbook of Aqueous Solubility Data: An Extensive Compilation of Aqueous Solubility Data for Organic Compounds Extracted from the AQUASOL dATAbASE. CRC Press LLC, Boca Raton, FL. 2003., p. 82

- **Hazardous Substances Data Bank (HSDB)**

Solubility in water, g/100ml at 20 °C: 13

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

13%

- **The National Institute for Occupational Safety and Health (NIOSH)**

3.2.8 Density

1.023 at 113 °F (NTP, 1992) - Denser than water; will sink

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

- **CAMEO Chemicals**

0.9867 g/cu cm @ 60 °C

Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 81st Edition. CRC Press LLC, Boca Raton: FL 2000, p. 3-92

- **Hazardous Substances Data Bank (HSDB)**

1.02 g/cm^3

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

0.99

- The National Institute for Occupational Safety and Health (NIOSH)

3.2.9 Vapor Density

2.1 (NTP, 1992) - Heavier than air; will sink (Relative to Air)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

- CAMEO Chemicals

2.8 (Air=1)

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 7D 3151

- Hazardous Substances Data Bank (HSDB)

Relative vapor density (air = 1): 2.1

- ILO-WHO International Chemical Safety Cards (ICSCs)

3.2.10 Vapor Pressure

2 mmHg at 392 °F (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

- CAMEO Chemicals

0.00778 [mmHg]

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

1.0382 Pa (0.00778 mm Hg) @ 298.29 K (25.14 °C) (solid)

Daubert, T.E., R.P. Danner. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, D.C.: Taylor and Francis, 1989.

- Hazardous Substances Data Bank (HSDB)

(212 °F): 2 mmHg

- The National Institute for Occupational Safety and Health (NIOSH)

3.2.11 LogP

log Kow = -0.99

PMID:4026577

Tanii H, Hashimoto K; Arch Toxicol 57: 88-93 (1985)

- Hazardous Substances Data Bank (HSDB)

-0.99

- ILO-WHO International Chemical Safety Cards (ICSCs)

3.2.12 Henry's Law Constant

Henry's Law constant = 6.5X10-9 atm-cu m/mol @ 25 °C /Estimated/

US EPA; Estimation Programs Interface (EPI). ver. 3.10. U.S. EPA version for Windows. Washington, DC: U.S. EPA (2001). Available from, as of Mar 1, 2004: https://www.epa.gov/oppt/exposure/pubs/episuitedl.htm

- Hazardous Substances Data Bank (HSDB)

3.2.13 Decomposition

After vacuum distillation of several tons of the nitrile at 150 C, lack of a receiver necessitated hot storage of the product at 80 C for 46 hours, and the drainage line blocked with solid. Though the bulk of the material was still liquid, heating to 195 C did not clear the line, and shortly afterwards decomposition occurred. It was subsequently found that the distillation residue had also decomposed at 175 C, 2 hours after distillation ended. Differntial thermal analysis showed that the nitrile is unusual in that no heat is evolved during the induction period of around 33 hours/200 C, or 1.5 hours/280 C, and the rapid onset and narrow peak width suggested a self-accelerating decomposition process, with Q = 700 J/g. No stabilising additives period for the nitrile to 20 percent of its value, while 1 percent of **potassium cyanide** reduced it to 2 percent.

Bretherick, L. Handbook of Reactive Chemical Hazards. 4th ed. Boston, MA: Butterworth-Heinemann Ltd., 1990, p. 425

- Hazardous Substances Data Bank (HSDB)

May be heated to 200 °C for 72 hr without decomposition.

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 1580

- **Hazardous Substances Data Bank (HSDB)**

3.2.14 Viscosity

0.002008 kg/m-sec @ 75 °C

Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 585

- **Hazardous Substances Data Bank (HSDB)**

3.2.15 Heat of Combustion

-2,285.38 kJ/mol

Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 585

- **Hazardous Substances Data Bank (HSDB)**

3.2.16 Heat of Vaporization

48.5 kJ/mol @ 266.0 °C

Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 585

- **Hazardous Substances Data Bank (HSDB)**

3.2.17 Surface Tension

0.04678 cu m/s @ 60 °C; 0.04572 cu m/s @ 70 °C; 0.04462cu m/s @ 80 °C

Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 585

- **Hazardous Substances Data Bank (HSDB)**

3.2.18 Odor Threshold

Odor perception threshold is 21 mg/L. Taste perception threshold is 200 mg/L.

Sheftel, V.O.; Indirect Food Additives and Polymers. Migration and Toxicology. Lewis Publishers, Boca Raton, FL. 2000., p. 1023

- **Hazardous Substances Data Bank (HSDB)**

3.2.19 Refractive Index

Index of refraction: 1.4173 D/ 60 °C

Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 81st Edition. CRC Press LLC, Boca Raton: FL 2000, p. 3-92

- **Hazardous Substances Data Bank (HSDB)**

3.2.20 Other Experimental Properties

Enthalpy of formation: 139.7 kJ/mol (liquid), 209.7 kJ/mol (gas); molar heat capacity: 145.6 J/K mol

Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 81st Edition. CRC Press LLC, Boca Raton: FL 2000, p. 5-35

- **Hazardous Substances Data Bank (HSDB)**

Enthalpy of fusion: 3.70 kJ/mol @ 57.98 °C

Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 81st Edition. CRC Press LLC, Boca Raton: FL 2000, p. 6-129

- **Hazardous Substances Data Bank (HSDB)**

Relative permittivity: 62.6 @ 298.2 K

Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 81st Edition. CRC Press LLC, Boca Raton: FL 2000, p. 6-154

- **Hazardous Substances Data Bank (HSDB)**

Conversion factor: 1 ppm = 3.28 mg/cu m; vapor pressure 2 mm Hg @ 212 °F (100 °C)

NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases. U.S. Department of Health & Human Services, Public Health Service, Center for Disease Control & Prevention. DHHS (NIOSH) Publication No. 2001-145 (CD-ROM) August 2001.

- **Hazardous Substances Data Bank (HSDB)**

Hydroxyl radical reaction rate constant = 4.3X10-14 cu cm/molecule-sec @ 25 °C /Estimated/

US EPA; Estimation Programs Interface (EPI). ver. 3.10. U.S. EPA version for Windows. Washington, DC: U.S. EPA (2001). Available from, as of Mar 1, 2004: ***https://www.epa.gov/oppt/exposure/pubs/episuitedl.htm***

- Hazardous Substances Data Bank (HSDB)

3.3 SpringerMaterials Properties

Schoenflies notation	Diffusion of impurities	Melting temperature	Preexpo
Activation energy	Diffusive flux	Migration energy	Quadrup
Boiling point	Formula unit	Molecular structure	Refractiv
Chemical bond	Fusion entropy	Nuclear magnetic resonance	Self-diffu
Chemical diffusion	Fusion temperature	Nuclear quadrupole resonance spectroscopy	Space gr
Creep	Grain size	Optical coefficient	Spin-latt
Crystal structure	Heat of sublimation	Partial pressure	Surface t
Density	Impurity concentration	Phase transition	Tracer di
Dielectric constant	Internuclear distance	Phonon wavenumber	Transitio
Diffusion	Isotope mass-effect	Point group	Tricritica

- SpringerMaterials

3.4 Chemical Classes

Nitrogen Compounds -> Nitriles

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

4 Spectral Information

4.1 1D NMR Spectra

1 of 2	
1D NMR Spectra	1H NMR: 10167 (Sadtler Research Laboratories Spectral Collection)

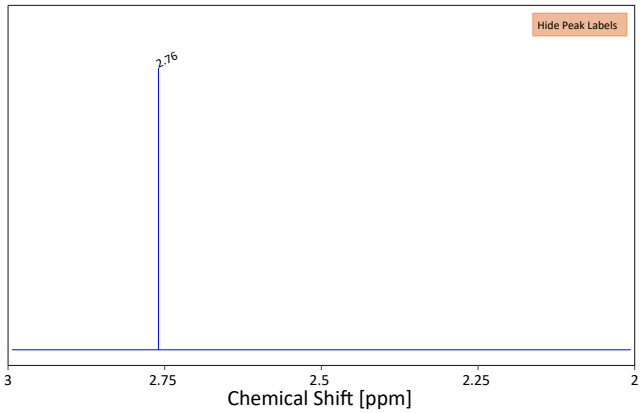
- Hazardous Substances Data Bank (HSDB)

2 of 2

1D NMR Spectra	NMRShiftDB Link

NMRShiftDB

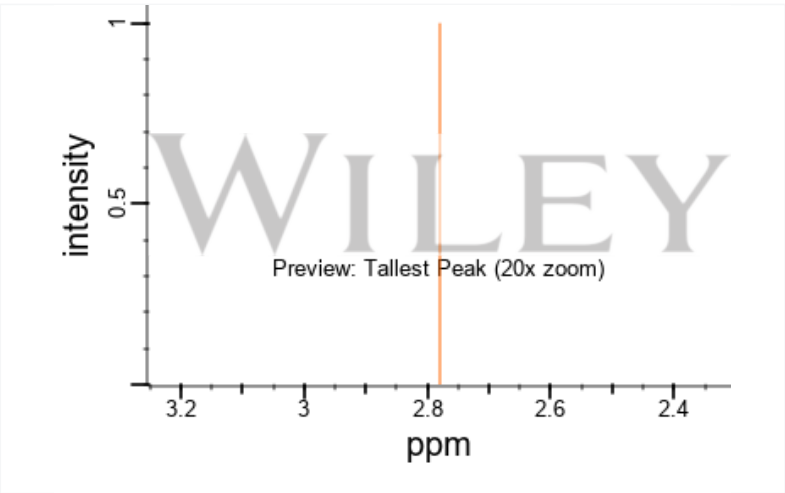
4.1.1 1H NMR Spectra

1 of 3	View All
Spectra ID	2144
Instrument Type	JEOL
Frequency	300 MHz
Solvent	CDCl3
Shifts [ppm]:Intensity	2.76:1000.00
Thumbnail	

Human Metabolome Database (HMDB)

2 of 3	View All
Instrument Name	Varian A-60
Copyright	Copyright © 2009-2024 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

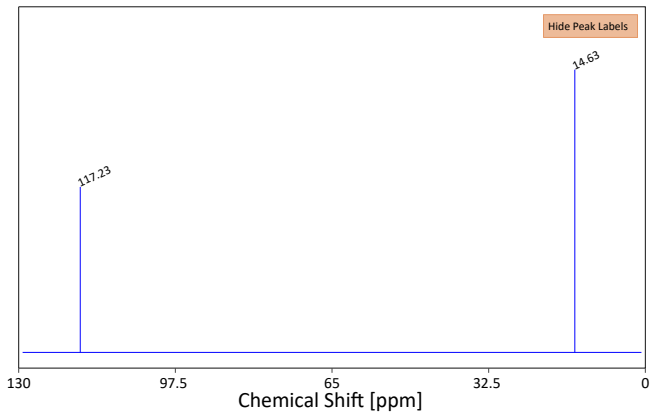


SpectraBase

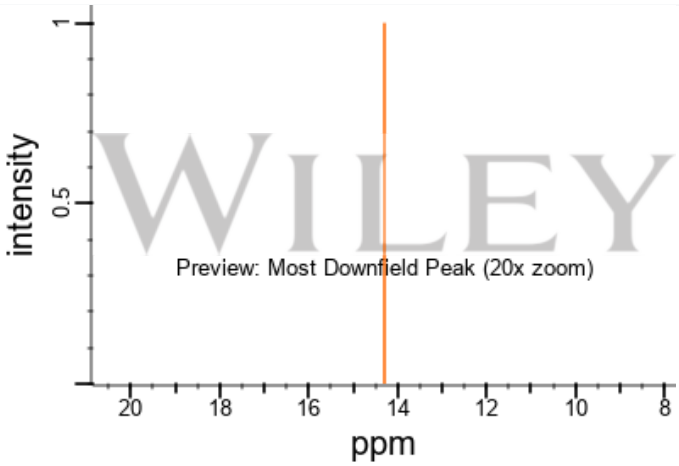
4.1.2 13C NMR Spectra

1 of 3 View All

Spectra ID	3451
Instrument Type	Varian
Frequency	25.16 MHz
Solvent	CDCl3
Shifts [ppm]:Intensity	117.23:585.00, 14.63:1000.00

Thumbnail	

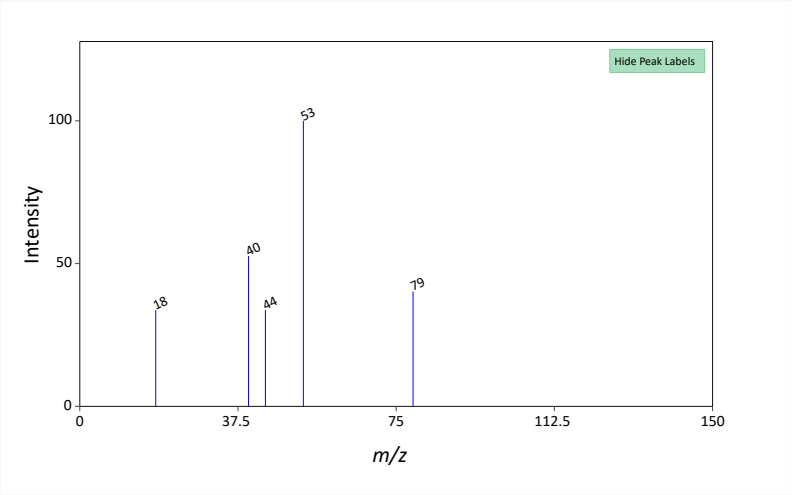
Human Metabolome Database (HMDB)

2 of 3	View All
Source of Sample	Aldrich Chemical Company, Inc., Milwaukee, Wisconsin
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

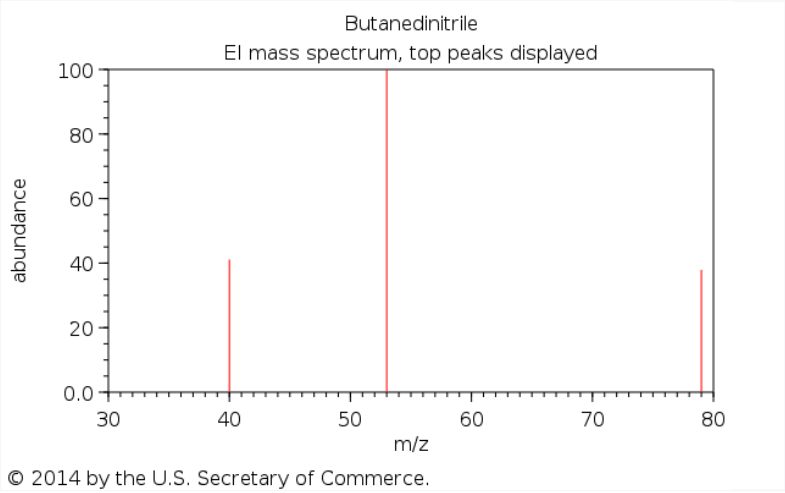
4.2 Mass Spectrometry

4.2.1 GC-MS

1 of 6	View All
MoNA ID	JP002890
MS Category	Experimental
MS Type	GC-MS
MS Level	MS1
Instrument	Unknown
Instrument Type	EI-B
Ionization Mode	positive
Top 5 Peaks	53 99.99 40 52.63 79 40.28 44 33.77 18 33.70
SPLASH	splash10-0ufu-9100000000-be8dd1d9da4b1e490786
Thumbnail	
License	CC BY-NC-SA

MassBank of North America (MoNA)

2 of 6	View All
NIST Number	341643

Library	Main library
Total Peaks	33
m/z Top Peak	53
m/z 2nd Highest	40
m/z 3rd Highest	79
Thumbnail	

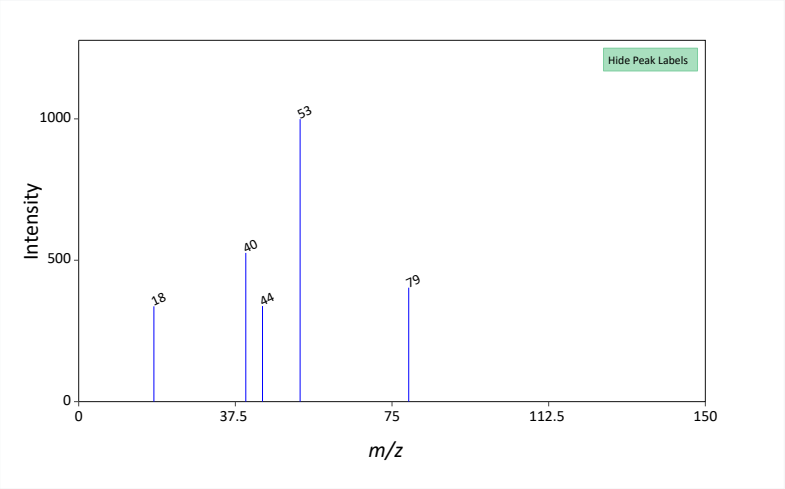
NIST Mass Spectrometry Data Center

4.2.2 Other MS

1 of 2	
Other MS	MASS: 50489 (NIST/EPA/MCMD Mass Spectral Database 1990 version)

Hazardous Substances Data Bank (HSDB)

2 of 2	
Accession ID	MSBNK-Fac_Eng_Univ_Tokyo-JP002890
Authors	MASS SPECTROSCOPY SOC. OF JAPAN (MSSJ)
Instrument	Unknown
Instrument Type	EI-B

MS Level	MS
Ionization Mode	POSITIVE
Top 5 Peaks	53 999 40 526 79 403 44 338 18 337
SPLASH	splash10-0ufu-9100000000-be8dd1d9da4b1e490786
Thumbnail	
License	CC BY-NC-SA

▸ MassBank Europe

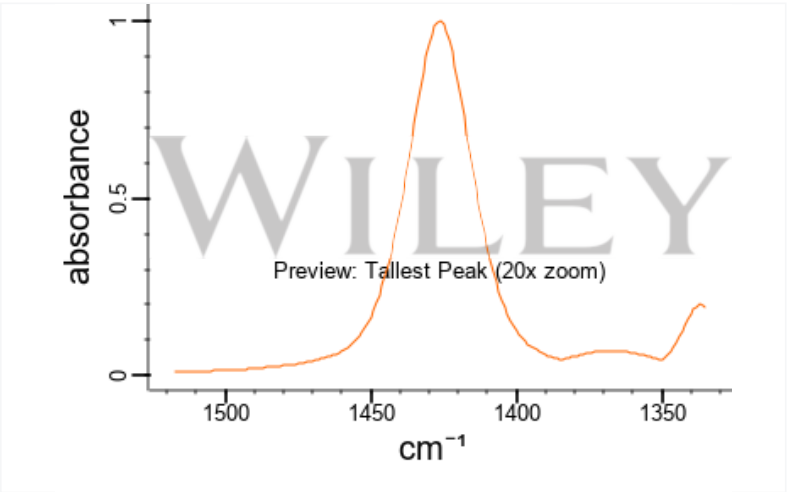
4.3 IR Spectra

IR Spectra	IR: 500 (Sadtler Research Laboratories IR prism collection)

▸ Hazardous Substances Data Bank (HSDB)

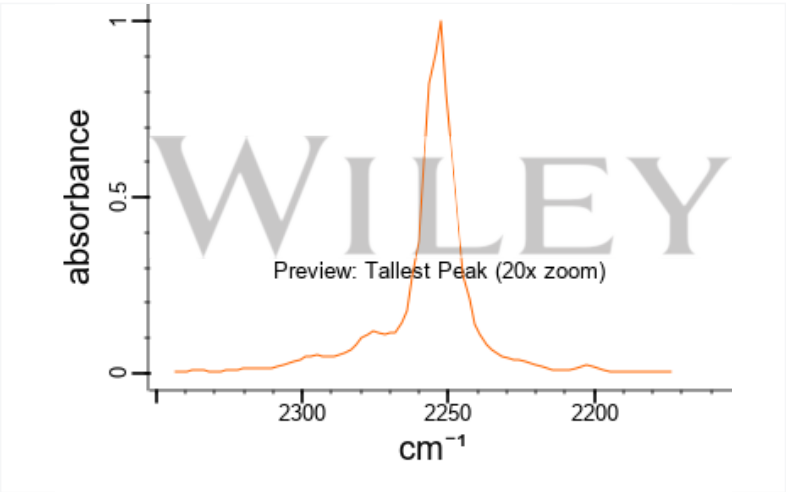
4.3.1 FTIR Spectra

1 of 2	
Instrument Name	Bruker IFS 85

Technique	Film
Source of Sample	Merck-Schuchardt Hohenbrunn
Copyright	Copyright © 1989, 1990-2024 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
Thumbnail	

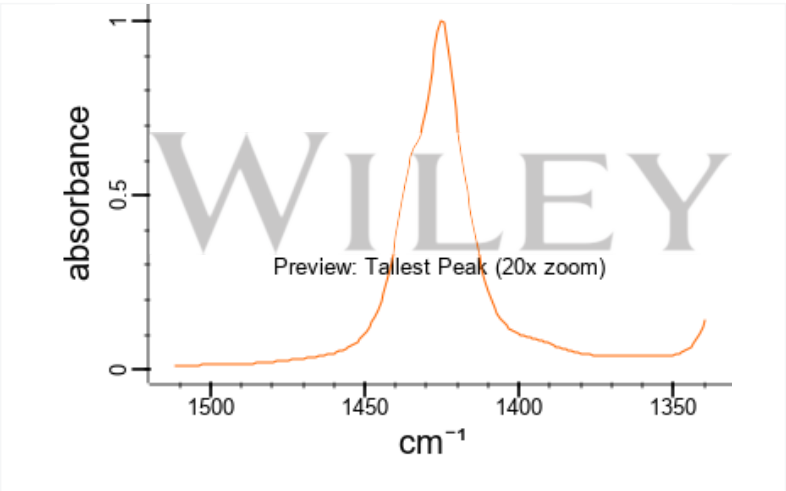
SpectraBase

2 of 2	
Instrument Name	Bruker IFS 85
Technique	Film
Copyright	Copyright © 1989, 1990-2024 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.

Thumbnail	

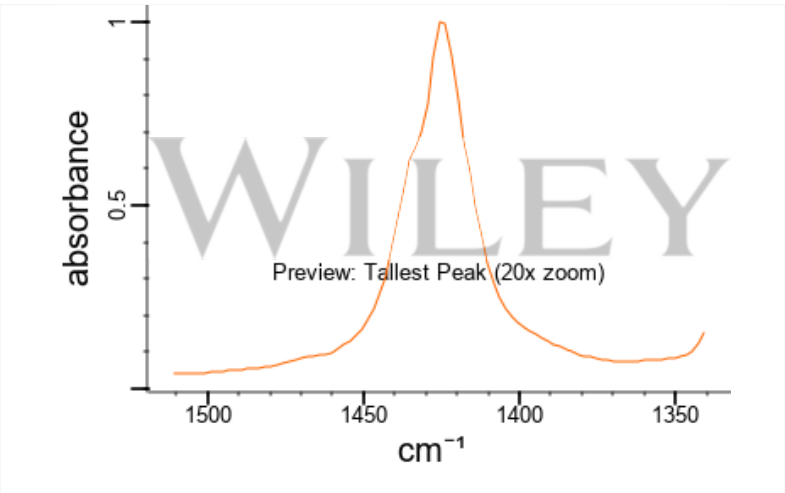
SpectraBase

4.3.2 ATR-IR Spectra

1 of 2	
Technique	ATR-Film
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

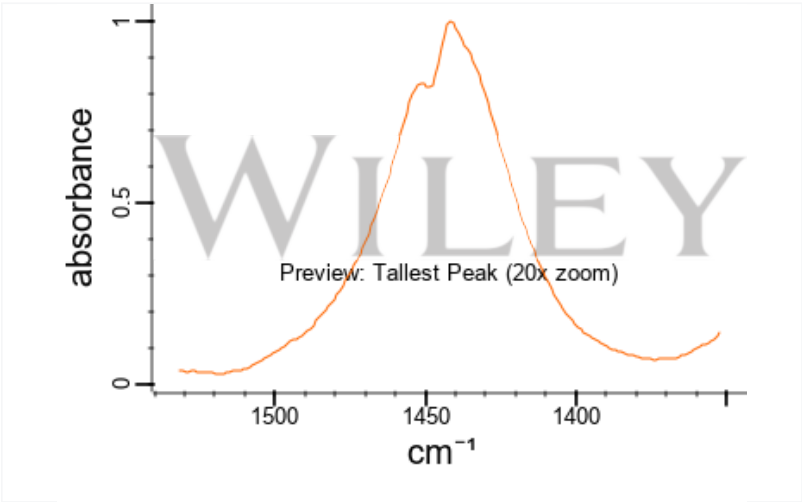
2 of 2

Source of Sample	Aldrich
Catalog Number	160962
Copyright	Copyright © 2018-2024 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2018-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

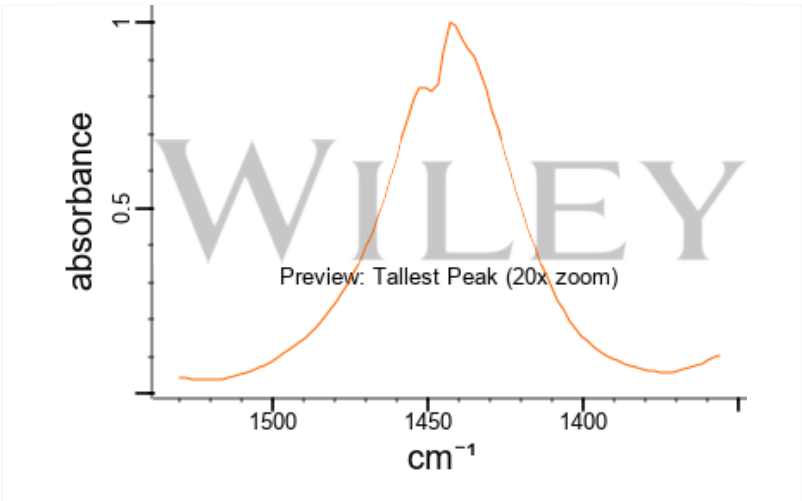
SpectraBase

4.3.3 Vapor Phase IR Spectra

1 of 2	
Instrument Name	DIGILAB FTS-14
Technique	Vapor Phase
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.

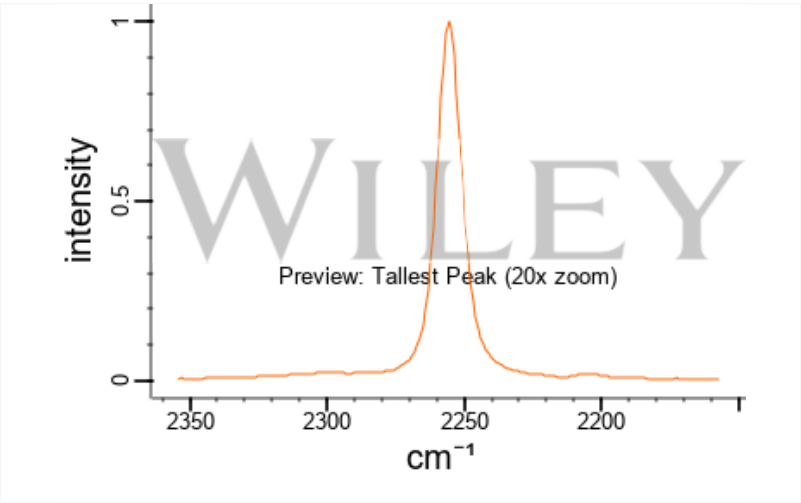
Thumbnail	

▸ SpectraBase

2 of 2	
Source of Spectrum	Sigma-Aldrich Co. LLC.
Source of Sample	Sigma-Aldrich Co. LLC.
Catalog Number	160962
Copyright	Copyright © 2021-2024 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

▸ SpectraBase

4.4 Raman Spectra

Catalog Number	160962
Copyright	Copyright © 2017-2024 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2017-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

- SpectraBase

5 Related Records

5.1 Related Compounds with Annotation

Follow these links to do a live 2D search or do a live 3D search for this compound, sorted by annotation score. This section is deprecated (see here for details), but these live search links provide equivalent functionality to the table that was previously shown here.

- PubChem

5.2 Related Compounds

Same Connectivity Count	7
Same Parent, Connectivity Count	12

Same Parent, Exact Count	6
Mixtures, Components, and Neutralized Forms Count	51
Similar Compounds (2D)	View in PubChem Search
Similar Conformers (3D)	View in PubChem Search

PubChem

5.3 Substances

5.3.1 PubChem Reference Collection SID

500829773

PubChem

5.3.2 Related Substances

All Count	223
Same Count	140
Mixture Count	83

PubChem

5.3.3 Substances by Category

PubChem

5.4 Entrez Crosslinks

PubMed Count	38

PubChem

6 Chemical Vendors

PubChem

7 Drug and Medication Information

7.1 Reported Fatal Dose

227 to 300 milligrams for an adult human (cyanide salts). (T86)

T86: Baselt RC and Cravey RH (1989). Disposition of Toxic Drugs and Chemicals in Man. 3rd ed. Chicago, IL.: Year Book Medical Publishers.

- **Toxin and Toxin Target Database (T3DB)**

8 Pharmacology and Biochemistry

8.1 Absorption, Distribution and Excretion

...The excretion of succinonitrile and its metabolites in urine and feces of mice, following a single injection of succinonitrile /was reported/. The cumulative excretion of succinonitrile and metabolites in urine and feces measured 60% by 24 hours and 83% by 72 hours. In the first multiple-dose experiment in which mice received three doses of unlabeled succinonitrile and one dose of radioactive succinonitrile, 52% of the radioactivity was excreted in urine in 24 hours. In the second multiple-dose experiment, in which mice received four doses of radioactive succinonitrile, 50% of the radioactivity was excreted in each 24 hr period.

U.S Department of Health, Education, and Welfare. Public Health Service. Center for Disease Control. National Institute for Occupational Safety and Health; NIOSH Criteria for a Recommended Standard - Occupational Exposure to Nitriles p.59 (September 1978) DHEW (NIOSH) Pub #78-212

- **Hazardous Substances Data Bank (HSDB)**

...The fate of 14C-labeled succinonitrile in male mice /was investigated/. ...A mean of 53% of the total succinonitrile injected ip in each animal in single and multiple dose studies was eliminated in the first 24 hours post-treatment and 88% of this eliminated succinonitrile was excreted as metabolites. In a single dose study, 7% of the 14C-labeled succinonitrile was excreted as **thiocyanate** and 36% as intermediate metabolites in 24 hours. In the multiple dose study, 18% **thiocyanate** and 24% intermediate metabolites were excreted.

U.S Department of Health, Education, and Welfare. Public Health Service. Center for Disease Control. National Institute for Occupational Safety and Health; NIOSH Criteria for a Recommended Standard - Occupational Exposure to Nitriles p.59 (September 1978) DHEW (NIOSH) Pub #78-212

- **Hazardous Substances Data Bank (HSDB)**

8.2 Metabolism / Metabolites

/A study/... determined that rats and rabbits converted about 60% of the succinonitrile to **cyanide**.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V4 1420

▸ Hazardous Substances Data Bank (HSDB)

...The release of **cyanide** from succinonitrile in rats and rabbits in vivo and in vitro /was investigated/. In the in vivo studies, male rabbits weighing 2-3 kg and male rats weighing 400-450 g were administered succinonitrile in iv doses of 25-40 mg/kg and 25-50 mg/kg, respectively. Levels of **cyanide** and **thiocyanate** were determined in samples of urine from rabbits and rats. The total number of rats that were studied was not mentioned. In the in vitro studies, levels of **cyanide** and **thiocyanate** were determined in liver slices and homogenates of rat or rabbit liver or with isolated mitochondrial, microsomal, and soluble fractions. Samples (0.1-2.0 mL) of filtered 24 hr urine output were collected form groups of two rats and from each rabbit pre- and post-administration with succinonitrile to determine **thiocyanate** concentrations. In another study, rats were pretreated with 2 mL/kg of **carbon tetrachloride** sc 48 hr prior to succinonitrile administration. Filtered urine samples were collected, and **cyanide** concentrations were determined colorimetrically. ...A sixfold increase in urinary **thiocyanate** following iv-injected doses of 25 mg/kg of succinonitrile /was found/ compared with the controls. Forty-eight to 120 hours postadministration of succinonitrile, **thiocyanate** levels approached control values. Pretreatment of rats by sc injection of 2 mL/kg **carbon tetrachloride** inhibited urinary **thiocyanate** excretion. Urinary excretion of **cyanide** increased over fivefold 48 hours posttreatment with succinonitrile. The values at 72-120 hours posttreatment approached normal values. ...Rat and rabbit liver slices catalyzed the release of **cyanide** from succinonitrile. However, 0.1-2.0 mg/g of Triton-**X-100** strongly inhibited **cyanide** release from succinonitrile in rat liver slices. Liver slices of rats pretreated with **carbon tetrachloride** did not release detectable amounts of **cyanide** for succinonitrile. .../It was/ concluded that rabbits and rats converted about 60% of the administered succinonitrile to **cyanide**, which was excreted as **thiocyanate**. The release of **cyanide** was inhibited by **carbon tetrachloride** and Triton-**X-100**. The authors also postulated that disruption of the liver cells, as by centrifugation to separate their contents, depressed or eliminated their ability to liberate **cyanide** ions or to form **thiocyanate**. The authors proposed that cellular membranes contain enzymes or enzyme complexes that are responsible for the conversion of succinonitrile to **cyanide**, which is excreted as **thiocyanate**. However, following homogenization, these enzyme or enzyme complexes may be destroyed or damaged by homogenization.

U.S Department of Health, Education, and Welfare. Public Health Service. Center for Disease Control. National Institute for Occupational Safety and Health; NIOSH Criteria for a Recommended Standard - Occupational Exposure to Nitriles p.58 (September 1978) DHEW (NIOSH) Pub #78-212

▸ Hazardous Substances Data Bank (HSDB)

/One study/ ...concluded that succinonitrile was either excreted unmetabolized or was metabolized to **cyanide** and excreted as **thiocyanate** in mice within 24 hours posttreatment. The authors postulated that the high percentage of metabolites excreted in 24 hr urine samples may be due to the presence of two reactive centres in the succinonitrile molecule,

resulting in the formation of two intermediate metabolites, diethylene cyanohydrin and **cyanoacetic acid**.

U.S Department of Health, Education, and Welfare. Public Health Service. Center for Disease Control. National Institute for Occupational Safety and Health; NIOSH Criteria for a Recommended Standard - Occupational Exposure to Nitriles p.58 (September 1978) DHEW (NIOSH) Pub #78-212

- **Hazardous Substances Data Bank (HSDB)**

The liberation of **cyanide** from succinonitrile has been studied to obtain information on the cellular systems responsible for the release of this metabolite. sing isolated endoplasmic reticulum preparations a complex between succinonitrile and cyt. P450 has been detected. This finding together with the inhibition of **cyanide** liberation by **SKF-525A** in liver slices indicates that the endoplasmic reticulum is involved in the early stages of succinonitrile metabolism. The decreased metabolism of succinonitrile which was observed after addition of inhibitors of oxidative phosphorylation indicates that an energy-dependent mitochondrial step might be involved in the subsequent steps. ...**Cyanide** liberation from succinonitrile is a multistep process in which the mitochondrial membrane and the endoplasmic reticulum are involved.

PMID:7274308

Floreani M et al; Eur J Drug Metab Pharmacokinet 6 (2): 135-40 (1981)

- **Hazardous Substances Data Bank (HSDB)**

Organic nitriles are converted into **cyanide** ions through the action of cytochrome P450 enzymes in the liver. **Cyanide** is rapidly absorbed and distributed throughout the body. **Cyanide** is mainly metabolized into **thiocyanate** by either rhodanese or **3-mercaptopyruvate sulfur** transferase. **Cyanide** metabolites are excreted in the urine. (L96)

L96: ATSDR - Agency for Toxic Substances and Disease Registry (2006). Toxicological profile for cyanide. U.S. Public Health Service in collaboration with U.S. Environmental Protection Agency (EPA). ***http://www.atsdr.cdc.gov/toxprofiles/tp8.html***

- **Toxin and Toxin Target Database (T3DB)**

8.3 Biological Half-Life

...The half-life of iv succinonitrile was calculated in both dogs and men to be about 21 hr.

Lodi F et al; Farmaco Ed Prat 28: 105-114 (1973)

- **Hazardous Substances Data Bank (HSDB)**

9 Use and Manufacturing

9.1 Uses

EPA CPDat Chemical and Product Categories

The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products, Scientific Data, volume 5, Article number: 180125 (2018), DOI:10.1038/sdata.2018.125

- EPA Chemical and Products Database (CPDat)

Sources/Uses

Used to make plastics and nitron fibers; [HSDB]

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

Used in the production of plastics and nitron fibers.

Sheftel, V.O.; Indirect Food Additives and Polymers. Migration and Toxicology. Lewis Publishers, Boca Raton, FL. 2000., p. 1023

- Hazardous Substances Data Bank (HSDB)

9.2 Methods of Manufacturing

Interaction of ethylene dibromide and potassium cyanide in the presence of alcohol.

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 467

- Hazardous Substances Data Bank (HSDB)

Succinonitrile is obtained by addition of **hydrogen cyanide** to **acrylonitrile**.

Ullmann's Encyclopedia of Industrial Chemistry. 6th ed.Vol 1: Federal Republic of Germany: Wiley-VCH Verlag GmbH & Co. 2003 to Present, p. V23 79 (2003)

- **Hazardous Substances Data Bank (HSDB)**

9.3 Formulations / Preparations

Trade names: deprelin, dinile, Suxil

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V4 1419

- **Hazardous Substances Data Bank (HSDB)**

9.4 General Manufacturing Information

EPA TSCA Commercial Activity Status

Butanedinitrile: ACTIVE

- **EPA Chemicals under the TSCA**

10 Identification

10.1 Analytic Laboratory Methods

... A colorimetric method for analyzing /air/ samples of succinonitrile, utilizing the pink-violet reaction products of succinonitrile nitro derivatives with alkali in a **toluene-acetone** medium followed by acidification of the solution. This method is sensitive to less than a microgram of succinonitrile in the final solution and provides a stable color for up to 30 minutes; however, nitro and halogenated aromatic hydrocarbons interfere with the determination.

U.S Department of Health, Education, and Welfare. Public Health Service. Center for Disease Control. National Institute for Occupational Safety and Health; NIOSH Criteria for a Recommended Standard - Occupational Exposure to Nitriles p.76 (September 1978) DHEW (NIOSH) Pub #78-212

- **Hazardous Substances Data Bank (HSDB)**

A mixture of **acrylonitrile**, **propionitrile**, **butyronitrile**, succinonitrile, and **adiponitrile** in an aqueous solution containing **hydrochloric acid** and **potassium chloride** was successfully analyzed by gas chromatography using a hot wire detector. However, gas chromatographic methods do not provide for specific determination of nitriles, and substances with similar

retention times may interfere. In the absence of interfering substances, nitriles may be separated and determined by comparison with appropriate standards.

U.S Department of Health, Education, and Welfare. Public Health Service. Center for Disease Control. National Institute for Occupational Safety and Health; NIOSH Criteria for a Recommended Standard - Occupational Exposure to Nitriles p.77 (September 1978) DHEW (NIOSH) Pub #78-212

- Hazardous Substances Data Bank (HSDB)

11 Safety and Hazards

11.1 Hazards Identification

11.1.1 GHS Classification

Pictogram(s)	Acute Toxic, Irritant, Environmental Hazard
Signal	Danger
GHS Hazard Statements	H302 (95%): Harmful if swallowed [**Warning** Acute toxicity, oral] H311 (36.2%): Toxic in contact with skin [**Danger** Acute toxicity, dermal] H315 (53.8%): Causes skin irritation [**Warning** Skin corrosion/irritation] H319 (53.8%): Causes serious eye irritation [**Warning** Serious eye damage/eye irritation] H335 (53.8%): May cause respiratory irritation [**Warning** Specific target organ toxicity, single exposure; Respiratory tract irritation] H400 (35%): Very toxic to aquatic life [**Warning** Hazardous to the aquatic environment, acute hazard] H410 (35%): Very toxic to aquatic life with long lasting effects [**Warning** Hazardous to the aquatic environment, long-term hazard]
Precautionary Statement Codes	P261, P262, P264, P264+P265, P270, P271, P273, P280, P301+P317, P302+P352, P304+P340, P305+P351+P338, P316, P319, P321, P330, P332+P317, P337+P317, P361+P364, P362+P364, P391, P403+P233, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided per 80 reports by companies from 12 notifications to the ECHA C&L Inventory. Each notification may be associated*

	with multiple companies. *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

▸ European Chemicals Agency (ECHA)

11.1.2 Hazard Classes and Categories

Acute Tox. 4 (95%)

Acute Tox. 3 (36.2%)

Skin Irrit. 2 (53.8%)

Eye Irrit. 2 (53.8%)

STOT SE 3 (53.8%)

Aquatic Acute 1 (35%)

Aquatic Chronic 1 (35%)

▸ European Chemicals Agency (ECHA)

11.1.3 NFPA Hazard Classification

NFPA 704 Diamond	 2-1-0
NFPA Health Rating	2 - Materials that, under emergency conditions, can cause temporary incapacitation or residual injury.
NFPA Fire Rating	1 - Materials that must be preheated before ignition can occur. Materials require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur.
NFPA Instability Rating	0 - Materials that in themselves are normally stable, even under fire conditions.

▸ Hazardous Substances Data Bank (HSDB)

11.1.4 Health Hazards

Excerpt from NIOSH Pocket Guide for Succinonitrile:

Exposure Routes: Inhalation, skin absorption, ingestion, skin and/or eye contact

Symptoms: Irritation eyes, skin, respiratory system; headache, dizziness, lassitude (weakness, exhaustion), confusion, convulsions; blurred vision; dyspnea (breathing difficulty); abdominal pain, nausea, vomiting

Target Organs: Eyes, skin, respiratory system, central nervous system, cardiovascular system (NIOSH, 2024)

- **CAMEO Chemicals**

11.1.5 Fire Hazards

This compound is combustible. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

- **CAMEO Chemicals**

Combustible. Gives off irritating or toxic fumes (or gases) in a fire.

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

11.1.6 Hazards Summary

Irritating to the eyes, skin, and respiratory tract; [Merck Index] See Nitriles.

Merck Index - O'Neil MJ, Heckelman PE, Dobbelaar PH, Roman KJ (eds). The Merck Index, An Encyclopedia of Chemicals, Drugs, and Biologicals, 15th Ed. Cambridge, UK: The Royal Society of Chemistry, 2013.

- **Haz-Map, Information on Hazardous Chemicals and Occupational Diseases**

11.1.7 Skin, Eye, and Respiratory Irritations

Potential symptoms of overexposure are irritation of eyes, skin, respiratory system... .

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 1580

- Hazardous Substances Data Bank (HSDB)

11.2 Safety and Hazard Properties

11.2.1 Flammable Limits

Flammability

Combustible Solid

- The National Institute for Occupational Safety and Health (NIOSH)

11.2.2 NIOSH Recommendations

Recommended Exposure Limit: 10 Hr Time-Weighted Avg: 6 ppm (20 mg/cu m).

NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases. U.S. Department of Health & Human Services, Public Health Service, Center for Disease Control & Prevention. DHHS (NIOSH) Publication No. 2001-145 (CD-ROM) August 2001.

- Hazardous Substances Data Bank (HSDB)

11.3 First Aid Measures

Inhalation First Aid

Fresh air, rest. Artificial respiration may be needed. Refer for medical attention.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Skin First Aid

Rinse skin with plenty of water or shower.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Eye First Aid

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Ingestion First Aid

Rinse mouth. Give a slurry of activated **charcoal** in **water** to drink. Do NOT induce vomiting. Refer for medical attention .

- **ILO-WHO International Chemical Safety Cards (ICSCs)**

11.3.1 First Aid

EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with **water** or **normal saline** solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician. IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop.

SKIN: IMMEDIATELY flood affected skin with **water** while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and **water**. If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment.

INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing.

INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of **water** to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport the victim to a hospital. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

- **CAMEO Chemicals**

(**See general first aid procedures**)

Eye: Irrigate immediately - If this chemical contacts the eyes, immediately wash (irrigate) the eyes with large amounts of **water**, occasionally lifting the lower and upper lids. Get medical attention immediately.

Skin: **Water** wash immediately - If this chemical contacts the skin, immediately wash the contaminated skin with **water**. If this chemical penetrates the clothing, immediately remove

the clothing and wash the skin with water. If symptoms occur after washing, get medical attention immediately.

Breathing: Respiratory support

Swallow: Medical attention immediately - If this chemical has been swallowed, get medical attention immediately.

- The National Institute for Occupational Safety and Health (NIOSH)

11.4 Fire Fighting

Fires involving this compound can be controlled with dry chemical, carbon dioxide or Halon extinguishers. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

- CAMEO Chemicals

Use water spray, powder, alcohol-resistant foam, carbon dioxide.

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.5 Accidental Release Measures

11.5.1 Isolation and Evacuation

Excerpt from ERG Guide 151 [Substances - Toxic (Non-Combustible)]:

IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids.

SPILL: Increase the immediate precautionary measure distance, in the downwind direction, as necessary.

FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

*2024 Emergency Response Guidebook, **https://www.phmsa.dot.gov/training/hazmat/erg/emergency-response-guidebook-erg***

- CAMEO Chemicals

11.5.2 Spillage Disposal

Ventilation. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Personal protection: particulate filter respirator adapted to the airborne concentration of the substance.

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.5.3 Disposal Methods

SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational exposure or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal, aquatic, and plant life; and conformance with environmental and public health regulations.

- Hazardous Substances Data Bank (HSDB)

11.5.4 Preventive Measures

SRP: Contaminated protective clothing should be segregated in such a manner so that there is no direct personal contact by personnel who handle, dispose, or clean the clothing. Quality assurance to ascertain the completeness of the cleaning procedures should be implemented before the decontaminated protective clothing is returned for reuse by the workers. Contaminated clothing should not be taken home at end of shift, but should remain at employee's place of work for cleaning.

- Hazardous Substances Data Bank (HSDB)

SRP: The scientific literature for the use of contact lenses in industry is conflicting. The benefit or detrimental effects of wearing contact lenses depend not only upon the substance, but also on factors including the form of the substance, characteristics and duration of the exposure, the uses of other eye protection equipment, and the hygiene of the lenses. However, there may be individual substances whose irritating or corrosive properties are such that the wearing of contact lenses would be harmful to the eye. In those specific cases, contact lenses should not be worn. In any event, the usual eye protection equipment should be worn even when contact lenses are in place.

- Hazardous Substances Data Bank (HSDB)

Adequate precautions should be taken against skin or eye contact.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V4 1420

- **Hazardous Substances Data Bank (HSDB)**

The worker should immediately wash the skin when it becomes contaminated.

NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases. U.S. Department of Health & Human Services, Public Health Service, Center for Disease Control & Prevention. DHHS (NIOSH) Publication No. 2001-145 (CD-ROM) August 2001.

- **Hazardous Substances Data Bank (HSDB)**

For more Preventive Measures (Complete) data for SUCCINONITRILE (6 total), please visit the **HSDB record page**.

- **Hazardous Substances Data Bank (HSDB)**

11.6 Handling and Storage

11.6.1 Nonfire Spill Response

SMALL SPILLS AND LEAKAGE: Should a spill occur while you are handling this chemical, you should dampen the solid spill material with alcohol, then transfer the dampened material to a suitable container. Use absorbent paper dampened with alcohol to pick up any remaining material. Seal the absorbent paper, and any of your clothes, which may be contaminated, in a vapor-tight plastic bag for eventual disposal. Solvent wash all contaminated surfaces with alcohol followed by washing with a strong soap and **water** solution. Do not reenter the contaminate area until the Safety Officer (or other responsible person) has verified that the area has been properly cleaned.

STORAGE PRECAUTIONS: You should store this material in a refrigerator. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

- **CAMEO Chemicals**

11.6.2 Safe Storage

Separated from strong oxidants, strong bases, strong acids, strong reducing agents and food and feedstuffs. Well closed.

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.7 Exposure Control and Personal Protection

11.7.1 Recommended Exposure Limit (REL)

TWA 6 ppm (20 mg/m^3)

- The National Institute for Occupational Safety and Health (NIOSH)

11.7.2 Permissible Exposure Limit (PEL)

none

- The National Institute for Occupational Safety and Health (NIOSH)

11.7.3 Immediately Dangerous to Life or Health (IDLH)

N.D.

See: IDLH INDEX

- The National Institute for Occupational Safety and Health (NIOSH)

11.7.4 Inhalation Risk

Evaporation at 20 °C is negligible; a harmful concentration of airborne particles can, however, be reached quickly when dispersed.

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.7.5 Effects of Short Term Exposure

The substance is irritating to the eyes, skin and respiratory tract. The substance may cause effects on the cellular respiration (inhibition). This may result in convulsions and respiratory failure. The effects may be delayed. Exposure at high levels could cause death.

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.7.6 Personal Protective Equipment (PPE)

Excerpt from NIOSH Pocket Guide for Succinonitrile:

Skin: PREVENT SKIN CONTACT - Wear appropriate personal protective clothing to prevent skin contact.

Eyes: PREVENT EYE CONTACT - Wear appropriate eye protection to prevent eye contact.

Wash skin: WHEN CONTAMINATED - The worker should immediately wash the skin when it becomes contaminated.

Remove: WHEN WET OR CONTAMINATED - Work clothing that becomes wet or significantly contaminated should be removed and replaced.

Change: DAILY - Workers whose clothing may have become contaminated should change into uncontaminated clothing before leaving the work premises.

Provide: EYEWASH - Eyewash fountains should be provided in areas where there is any possibility that workers could be exposed to the substances; this is irrespective of the recommendation involving the wearing of eye protection. (NIOSH, 2024)

- **CAMEO Chemicals**

Respirator Recommendations: Up to 60 ppm: (Assigned protection factor = 10) Any supplied-air respirator.

NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases. U.S. Department of Health & Human Services, Public Health Service, Center for Disease Control & Prevention. DHHS (NIOSH) Publication No. 2001-145 (CD-ROM) August 2001.

- **Hazardous Substances Data Bank (HSDB)**

Respirator Recommendations: Up to 150 ppm: (Assigned protection factor = 25) Any supplied-air respirator operated in a continuous-flow mode.

NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases. U.S. Department of Health & Human Services, Public Health Service, Center for Disease Control & Prevention. DHHS (NIOSH) Publication No. 2001-145 (CD-ROM) August 2001.

- **Hazardous Substances Data Bank (HSDB)**

Respirator Recommendations: Up to 250 ppm: (Assigned protection factor = 50) Any self-contained breathing apparatus with a full facepiece/(Assigned protection factor = 50) Any supplied-air respirator with a full facepiece.

NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases. U.S. Department of Health & Human Services, Public Health Service, Center for Disease Control & Prevention. DHHS (NIOSH) Publication No. 2001-145 (CD-ROM) August 2001.

- Hazardous Substances Data Bank (HSDB)

Respirator Recommendations: Emergency or planned entry into unknown concentrations or IDLH conditions: (Assigned protection factor = 10,000) Any self-contained breathing apparatus that has a full facepiece and is operated in a pressure-demand or other positive-pressure mode/(Assigned protection factor = 10,000) Any supplied-air respirator that has a full facepiece and is operated in a pressure-demand or other positive-pressure mode in combination with an auxiliary self-contained positive-pressure breathing apparatus.

NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases. U.S. Department of Health & Human Services, Public Health Service, Center for Disease Control & Prevention. DHHS (NIOSH) Publication No. 2001-145 (CD-ROM) August 2001.

- Hazardous Substances Data Bank (HSDB)

For more Personal Protective Equipment (PPE) (Complete) data for SUCCINONITRILE (8 total), please visit the **HSDB record page**.

- Hazardous Substances Data Bank (HSDB)

(**See personal protection and sanitation codes**)

Skin: Prevent skin contact - Wear appropriate personal protective clothing to prevent skin contact.

Eyes: Prevent eye contact - Wear appropriate eye protection to prevent eye contact.

Wash skin: When contaminated

Remove: When wet or contaminated

Change: Daily - Workers whose clothing may have become contaminated should change into uncontaminated clothing before leaving the work premises.

Provide: Eyewash - Eyewash fountains should be provided in areas where there is any possibility that workers could be exposed to the substances; this is irrespective of the recommendation involving the wearing of eye protection.

- The National Institute for Occupational Safety and Health (NIOSH)

11.7.7 Respirator Recommendations

NIOSH

Up to 60 ppm:

(APF = 10) Any supplied-air respirator

Up to 150 ppm:

(APF = 25) Any supplied-air respirator operated in a continuous-flow mode

Up to 250 ppm:

(APF = 50) Any self-contained breathing apparatus with a full facepiece

(APF = 50) Any supplied-air respirator with a full facepiece

Emergency or planned entry into unknown concentrations or IDLH conditions:

(APF = 10,000) Any self-contained breathing apparatus that has a full facepiece and is operated in a pressure-demand or other positive-pressure mode

(APF = 10,000) Any supplied-air respirator that has a full facepiece and is operated in a pressure-demand or other positive-pressure mode in combination with an auxiliary self-contained positive-pressure breathing apparatus

Escape:

(APF = 50) Any air-purifying, full-facepiece respirator (gas mask) with a chin-style, front- or back-mounted organic vapor canister

Any appropriate escape-type, self-contained breathing apparatus

Important additional information about respirator selection

- The National Institute for Occupational Safety and Health (NIOSH)

11.7.8 Preventions

Fire Prevention

NO open flames.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Exposure Prevention

PREVENT DISPERSION OF DUST!

- ILO-WHO International Chemical Safety Cards (ICSCs)

Inhalation Prevention

Use local exhaust or breathing protection.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Skin Prevention

Protective gloves.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Eye Prevention

Wear safety goggles.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Ingestion Prevention

Do not eat, drink, or smoke during work. Wash hands before eating.

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.8 Stability and Reactivity

11.8.1 Air and Water Reactions

Soluble in water [Hawley].

- CAMEO Chemicals

11.8.2 Reactive Group

Nitriles

- CAMEO Chemicals

11.8.3 Reactivity Profile

SUCCINONITRILE is incompatible with acids and oxidizing agents (such as peroxides and epoxides). Can react violently with strong oxidizing acids. Is hydrolyzed exothermically in both aqueous acid and base to give carboxylic acids (or salts of carboxylic acids). Can react vigorously with reducing agents.

- CAMEO Chemicals

11.8.4 Hazardous Reactivities and Incompatibilities

Oxidizers

NIOSH. NIOSH Pocket Guide to Chemical Hazards & Other Databases. U.S. Department of Health & Human Services, Public Health Service, Center for Disease Control & Prevention. DHHS (NIOSH) Publication No. 2001-145 (CD-ROM) August 2001.

- Hazardous Substances Data Bank (HSDB)

11.9 Transport Information

11.9.1 DOT Label

Poison

- CAMEO Chemicals

11.9.2 Packaging and Labelling

Do not transport with food and feedstuffs.

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.9.3 UN Classification

UN Hazard Class: 6.1; UN Pack Group: III

- ILO-WHO International Chemical Safety Cards (ICSCs)

11.10 Regulatory Information

The Australian Inventory of Industrial Chemicals

Chemical: Butanedinitrile

- Australian Industrial Chemicals Introduction Scheme (AICIS)

REACH Registered Substance

Status: Active Update: 25-11-2021 https://echa.europa.eu/registration-dossier/-/registered-dossier/21898

- European Chemicals Agency (ECHA)

New Zealand EPA Inventory of Chemical Status

Succinodinitrile: Does not have an individual approval but may be used under an appropriate group standard

- New Zealand Environmental Protection Authority (EPA)

11.10.1 Atmospheric Standards

This action promulgates standards of performance for equipment leaks of Volatile Organic Compounds (VOC) in the Synthetic Organic Chemical Manufacturing Industry (SOCMI). The intended effect of these standards is to require all newly constructed, modified, and reconstructed SOCMI process units to use the best demonstrated system of continuous emission reduction for equipment leaks of VOC, considering costs, non air quality health and environmental impact and energy requirements. Succinonitrile is produced, as an intermediate or a final product, by process units covered under this subpart.

*40 CFR 60.489; U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of February 10, 2004: **https://www.ecfr.gov***

- Hazardous Substances Data Bank (HSDB)

12 Toxicity

12.1 Toxicological Information

12.1.1 Toxicity Summary

Organic nitriles decompose into **cyanide** ions both in vivo and in vitro. Consequently the primary mechanism of toxicity for organic nitriles is their production of toxic **cyanide** ions or **hydrogen cyanide**. **Cyanide** is an inhibitor of cytochrome c oxidase in the fourth complex of the electron transport chain (found in the membrane of the mitochondria of eukaryotic cells). It complexes with the **ferric iron** atom in this enzyme. The binding of **cyanide** to this cytochrome prevents transport of electrons from cytochrome c oxidase to **oxygen**. As a result, the electron transport chain is disrupted and the cell can no longer aerobically produce **ATP** for energy. Tissues that mainly depend on aerobic respiration, such as the central nervous system and the heart, are particularly affected. **Cyanide** is also known produce some of its toxic effects by binding to catalase, **glutathione** peroxidase, methemoglobin, **hydroxocobalamin**, phosphatase, tyrosinase, **ascorbic acid** oxidase, **xanthine** oxidase, succinic dehydrogenase, and Cu/Zn superoxide dismutase. **Cyanide** binds to the **ferric** ion of methemoglobin to form inactive cyanmethemoglobin. (L97)

*L97: Wikipedia. Cyanide poisoning. Last Updated 30 March 2009. **http://en.wikipedia.org/wiki/Cyanide_poisoning***

- Toxin and Toxin Target Database (T3DB)

12.1.2 NIOSH Toxicity Data

- The National Institute for Occupational Safety and Health (NIOSH)

12.1.3 Carcinogen Classification

Carcinogen Classification	No indication of carcinogenicity to humans (not listed by IARC).

- Toxin and Toxin Target Database (T3DB)

12.1.4 Health Effects

Exposure to high levels of **cyanide** for a short time harms the brain and heart and can even cause coma, seizures, apnea, cardiac arrest and death. Chronic inhalation of **cyanide** causes breathing difficulties, chest pain, vomiting, blood changes, headaches, and enlargement of the thyroid gland. Skin contact with cyanide salts can irritate and produce sores. (L96, L97)

L96: ATSDR - Agency for Toxic Substances and Disease Registry (2006). Toxicological profile for cyanide. U.S. Public Health Service in collaboration with U.S. Environmental Protection Agency (EPA). ***http://www.atsdr.cdc.gov/toxprofiles/tp8.html***

L97: Wikipedia. Cyanide poisoning. Last Updated 30 March 2009. ***http://en.wikipedia.org/wiki/Cyanide_poisoning***

- Toxin and Toxin Target Database (T3DB)

12.1.5 Exposure Routes

The substance can be absorbed into the body by ingestion and by inhalation.

- ILO-WHO International Chemical Safety Cards (ICSCs)

inhalation, skin absorption, ingestion, skin and/or eye contact

- The National Institute for Occupational Safety and Health (NIOSH)

Oral (L96) ; inhalation (L96) ; dermal (L96)

L96: ATSDR - Agency for Toxic Substances and Disease Registry (2006). Toxicological profile for cyanide. U.S. Public Health Service in collaboration with U.S. Environmental Protection Agency (EPA). ***http://www.atsdr.cdc.gov/toxprofiles/tp8.html***

- Toxin and Toxin Target Database (T3DB)

12.1.6 Symptoms

Inhalation Exposure

Cough. Sore throat. Dizziness. Headache. Nausea. Convulsions.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Skin Exposure

Redness. Pain.

- ILO-WHO International Chemical Safety Cards (ICSCs)

Ingestion Exposure

Abdominal pain. Diarrhoea. Headache. Nausea. Vomiting. Convulsions.

- ILO-WHO International Chemical Safety Cards (ICSCs)

irritation eyes, skin, respiratory system; headache, dizziness, lassitude (weakness, exhaustion), confusion, convulsions; blurred vision; dyspnea (breathing difficulty); abdominal pain, nausea, vomiting

- The National Institute for Occupational Safety and Health (NIOSH)

Cyanide poisoning is identified by rapid, deep breathing and shortness of breath, general weakness, giddiness, headaches, vertigo, confusion, convulsions/seizures and eventually loss of consciousness. (L96, L97)

L96: ATSDR - Agency for Toxic Substances and Disease Registry (2006). Toxicological profile for cyanide. U.S. Public Health Service in collaboration with U.S. Environmental Protection Agency (EPA). ***http://www.atsdr.cdc.gov/toxprofiles/tp8.html***

L97: Wikipedia. Cyanide poisoning. Last Updated 30 March 2009. ***http://en.wikipedia.org/wiki/Cyanide_poisoning***

- **Toxin and Toxin Target Database (T3DB)**

12.1.7 Target Organs

Eyes, skin, respiratory system, central nervous system, cardiovascular system

- **The National Institute for Occupational Safety and Health (NIOSH)**

12.1.8 Adverse Effects

Other Poison - Chemical Asphyxiant

- **Haz-Map, Information on Hazardous Chemicals and Occupational Diseases**

12.1.9 Acute Effects

- ChemIDplus

12.1.10 Toxicity Data

LCLo (rat) = 730 mg/m3/4h

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

LD50: 450 mg/kg (Oral, Rat) (T29)

T29: Bingham, E, Cohrssen, B, and Powell, CH (2001). Patty's Toxicology Volumes 1-9. 5th ed. New York, N.Y: John Wiley & Sons.

- Toxin and Toxin Target Database (T3DB)

12.1.11 Treatment

Antidotes to cyanide poisoning include hydroxocobalamin and sodium nitrite, which release the cyanide from the cytochrome system, and rhodanase, which is an enzyme occurring naturally in mammals that combines serum cyanide with thiosulfate, producing comparatively harmless thiocyanate. Oxygen therapy can also be administered. (L97)

L97: Wikipedia. Cyanide poisoning. Last Updated 30 March 2009.
http://en.wikipedia.org/wiki/Cyanide_poisoning

- Toxin and Toxin Target Database (T3DB)

12.1.12 Antidote and Emergency Treatment

Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilation if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Administer amyl nitrite ampules as per protocol and physician order ... . Monitor for shock and treat if necessary ... . Monitor for pulmonary edema and treat if necessary ... . Anticipate seizures and treat if necessary ... . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline during transport ... . Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool ... . /Cyanide and related compounds/

Bronstein, A.C., P.L. Currance; Emergency Care for Hazardous Materials Exposure. 2nd ed. St. Louis, MO. Mosby Lifeline. 1994., p. 387-8

▸ Hazardous Substances Data Bank (HSDB)

Advanced treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious or in respiratory arrest. Positive pressure ventilation techniques with a bag valve mask device may be beneficial. Start an IV with D5W /SRP: "To keep open", minimal flow rate/. Use lactated Ringer's if signs of hypovolemia are present. Watch for signs of fluid overload. Administer **cyanide** antidote kit as per protocol and physician order ... . Monitor and treat cardiac arrhythmias if necessary ... . Consider vasopressors to treat hypotension without signs of hypovolemia ... . Consider drug therapy for pulmonary edema ... . Treat seizures with **diazepam** ... . Use **proparacaine hydrochloride** to assist eye irrigation ... . /**Cyanide** and related compounds/

Bronstein, A.C., P.L. Currance; Emergency Care for Hazardous Materials Exposure. 2nd ed. St. Louis, MO. Mosby Lifeline. 1994., p. 388

▸ Hazardous Substances Data Bank (HSDB)

12.1.13 Medical Surveillance

Medical surveillance should include pre-employment and periodic examinations focused on skin disorders and the cardiovascular, pulmonary and central nervous systems. A history of fainting spells or convulsive disorders might present an added risk for nitrile workers. /Nitriles/

International Labour Office. Encyclopaedia of Occupational Health and Safety. 4th edition, Volumes 1-4 1998. Geneva, Switzerland: International Labour Office, 1998., p. 104.134

▸ Hazardous Substances Data Bank (HSDB)

12.1.14 Human Toxicity Excerpts

/SIGNS AND SYMPTOMS/ Exposure to toxic nitriles may rapidly cause death by asphyxiation similar to that resulting from exposure to **hydrogen cyanide**. Individuals who survived exposure to high concentrations of nitriles were said to have no evidence of residual physiological effects after the recovery from the acute episode; this has led to the opinion that the person either succumbs to the nitrile exposure or recovers completely. /Nitriles/

International Labour Office. Encyclopaedia of Occupational Health and Safety. 4th edition, Volumes 1-4 1998. Geneva, Switzerland: International Labour Office, 1998., p. 104.134

▸ Hazardous Substances Data Bank (HSDB)

/SIGNS AND SYMPTOMS/ Potential symptoms of overexposure are irritation of eyes, skin, respiratory system; headache, dizziness, weakness, giddiness, confusion, convulsions; blurred

vision; dyspnea; abdominal pain, nausea, vomiting.

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 1580

- **Hazardous Substances Data Bank (HSDB)**

/CASE REPORTS/ A 53 yr old male with polyarthritis and chronic bronchitis had been treated for 3 weeks with anti-catarrhal drugs, vitamins, and a daily intramuscular injection of 200 mg succinonitrile. Two hours after the last injection, the patient began vomiting and showed signs of psychomotor agitation and mental confusion accompanied by cold sweating. He was admitted to a hospital with convulsions and mental disorientation. The patient died 2 hours after he was hospitalized during a convulsion. Autopsy showed pronounced visceral congestion and cerebral and pulmonary edema. Histological examination showed a massive and vacuolar hepatic degeneration and a significant nephrosis of the tubules. Because of the odor of bitter almonds when the skull was opened, a chemical analysis for **cyanide** compounds was conducted. **Cyanide** concentrations of 0.265 to 1.500 mg/100 mL, reported as **potassium-cyanide**, were found in the liver, brain, kidney, lungs, and urine. No evidence of **cyanide** was found in the blood or gastric contents. An ampule of the pharmaceutical product containing the succinonitrile was analyzed. No trace of **cyanide** was found. .../It was concluded/ that death was due to **cyanide** poisoning, the **cyanide** having accumulated in the body as a result of a metabolic disorder when succinonitrile was administered.

Marigo M et al; Medicina Legale e delle Assicurazioni 14: 1444-185 (1900)

- **Hazardous Substances Data Bank (HSDB)**

12.1.15 Non-Human Toxicity Excerpts

/LABORATORY ANIMALS: Acute Exposure/ The effects on the skin of rabbits of a 95% **water** solution were those of mild irritation. Continued contact of the solution with rabbit skin for 18 hr produced fatalities, indicating a probably hazard by skin absorption.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V4 1420

- **Hazardous Substances Data Bank (HSDB)**

/LABORATORY ANIMALS: Acute Exposure/ A 24 hr exposure of mice to vapor from a 95% solution caused no symptoms.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V4 1420

- **Hazardous Substances Data Bank (HSDB)**

/LABORATORY ANIMALS: Acute Exposure/ Administration of high doses is accompanied /by/ an increase in concentration of rhodanides in the urine. Animals exhibit general inhibition, impaired respiration, and exophthalmos with subsequent convulsions and death from respiratory arrest. Gross pathology examination revealed marked congestion in the brain and all visceral organs.

Sheftel, V.O.; Indirect Food Additives and Polymers. Migration and Toxicology. Lewis Publishers, Boca Raton, FL. 2000., p. 1023

- **Hazardous Substances Data Bank (HSDB)**

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ Guinea pigs were gavaged with 1/5 and 1/20 LD50 (120 mg/kg bw) for 75 days. The treatment resulted in decreased CO2 expiration, leukopenia, reduced leukocyte phagocytic activity and an increase in the **ascorbic acid** contents in the liver, kidneys, and suprarenals. Gross pathology examination revealed parenchymatous dystrophy in the visceral organs, circulatory disturbances, and a reduction in the spleen relative weights.

Sheftel, V.O.; Indirect Food Additives and Polymers. Migration and Toxicology. Lewis Publishers, Boca Raton, FL. 2000., p. 1023

- **Hazardous Substances Data Bank (HSDB)**

For more Non-Human Toxicity Excerpts (Complete) data for SUCCINONITRILE (6 total), please visit the **HSDB record page**.

- **Hazardous Substances Data Bank (HSDB)**

12.1.16 Non-Human Toxicity Values

LD50 Rat oral 450 mg/kg

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V4 1420

- **Hazardous Substances Data Bank (HSDB)**

12.2 Ecological Information

12.2.1 ICSC Environmental Data

Environmental effects from the substance have not been investigated adequately.

- ILO-WHO International Chemical Safety Cards (ICSCs)

12.2.2 Environmental Fate / Exposure Summary

Aliphatic nitriles such as succinonitrile are important starting materials for polymers, and the synthesis of pharmaceuticals and pesticides. Succinonitrile's production and use may result in its release to the environment through various waste streams. If released to air, a vapor pressure of 0.00778 mm Hg at 25 °C indicates succinonitrile will exist solely as a vapor in the ambient atmosphere. The reaction of vapor-phase succinonitrile with photochemically-produced hydroxyl radicals is not expected to be an important environmental fate process based on the estimated half-life for this reaction in air of 380 days. Succinonitrile is not expected to be susceptible to direct photolysis by sunlight, since it does not contain functional groups that are expected to absorb light with wavelengths >290 nm. If released to soil, succinonitrile is expected to have very high mobility based upon an estimated Koc of 28. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 5.1X10-9 atm-cu m/mole. Succinonitrile is not expected to volatilize from dry soil surfaces based upon its vapor pressure. In studies with activated sludge, biodegradation of 1.5-3.8% was observed after 6-24 hours. These studies suggest that succinonitrile may have been toxic to the microorganisms, since a high concentration of succinonitrile was used. If released into **water**, succinonitrile is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from **water** surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. An estimated BCF of 3 suggests the potential for bioconcentration in aquatic organisms is low. Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions. Occupational exposure to succinonitrile may occur through inhalation and dermal contact with this compound at workplaces where succinonitrile is produced or used. (SRC)

- Hazardous Substances Data Bank (HSDB)

12.2.3 Artificial Pollution Sources

Aliphatic nitriles, such as succinonitrile, are important starting materials for polymers, and the synthesis of pharmaceuticals and pesticides(1). Succinonitrile's production and use may result in its release to the environment through various waste streams(SRC).

(1) Pollak P et al; in Ullmann's Encycl Indust Chem. 5th ed. Gerhartz W, ed. Deerfield Beach, FL: VCH Pub, A17: 363-376 (1991)

▸ Hazardous Substances Data Bank (HSDB)

12.2.4 Environmental Fate

TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 28(SRC), determined from a structure estimation method(2), indicates that succinonitrile is expected to have very high mobility in soil(SRC). Volatilization of succinonitrile from moist soil surfaces is not expected to be an important fate process(SRC) given an estimated Henry's Law constant of 6.5X10-9 atm-cu m/mole(SRC), derived from its vapor pressure, 0.00778 mm Hg(3), and **water** solubility, 126.9 g/L(4). Succinonitrile is not expected to volatilize from dry soil surfaces(SRC) based upon a vapor pressure of 0.00778 mm Hg(3). In studies with activated sludge, biodegradation of 1.5-3.8% was observed after 6-24 hours(5). These studies suggest that succinonitrile may have been toxic to the microorganisms, since a high concentration of succinonitrile was used(5).

(1) Swann RL et al; Res Rev 85: 17-28 (1983)

(2) Meylan WM et al; Environ Sci Technol 26: 1560-67 (1992)

(3) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, DC: Taylor and Francis (1989)

(4) Yalkowsky SH, He Y, eds; Handbook of Aqueous Solubility Data. Boca Raton, FL: CRC Press LLC, p. 82 (2003)

(5) Malaney GW, Gerhold RM; J Water Pollut Control Fed 4: R18-R33 (1969)

▸ Hazardous Substances Data Bank (HSDB)

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 28(SRC), determined from a structure estimation method(2), indicates that succinonitrile is not expected to adsorb to suspended solids and sediment(SRC). Volatilization from **water** surfaces is not expected(3) based upon an estimated Henry's Law constant of 6.5X10-9 atm-cu m/mole(SRC), derived from its vapor pressure, 0.00778 mm Hg(4) and **water** solubility, 126.9 g/L(5). According to a classification scheme(6), an estimated BCF of 3(SRC), from its log Kow of -0.99(7) and a regression-derived equation(8), suggests the potential for bioconcentration in aquatic organisms is low(SRC). Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions(9). In studies with activated sludge, biodegradation of 1.5-3.8% was observed after 6-24 hours(10). These studies suggest that succinonitrile may have been toxic to the microorganisms, since a high concentration of succinonitrile was used(10).

(1) Swann RL et al; Res Rev 85: 17-28 (1983)

(2) Meylan WM et al; Environ Sci Technol 26: 1560-67 (1992)

(3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9, 15-1 to 15-29 (1990)

(4) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, DC: Taylor and Francis (1989)

(5) Yalkowsky SH, He Y, eds; Handbook of Aqueous Solubility Data. Boca Raton, FL: CRC Press LLC, p. 82 (2003)

(6) Franke C et al; Chemosphere 29: 1501-14 (1994)

(7) Tanii H, Hashimoto K; Arch Toxicol 57: 88-93 (1985)

(8) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999)

(9) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 7-4, 7-5 (1990)

(10) Malaney GW, Gerhold RM; J Water Pollut Control Fed 4: R18-R33 (1969)

Hazardous Substances Data Bank (HSDB)

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), succinonitrile, which has a vapor pressure of 0.00778 mm Hg at 25 °C(2), is expected to exist solely as a vapor in the ambient atmosphere. The reaction of vapor-phase succinonitrile with photochemically-produced hydroxyl radicals is not expected to be an important environmental fate based on the estimated half-life for this reaction in air of 380 days, calculated from its rate constant of 4.3X10-14 cu cm/molecule-sec at 25 deg (SRC) that was derived using a structure estimation method(3). Succinonitrile is not expected to be susceptible to direct photolysis by sunlight, since it does not contain functional groups that are expected to absorb light with wavelengths >290 nm(SRC).

(1) Bidleman TF; Environ Sci Technol 22: 361-367 (1988)

(2) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, DC: Taylor and Francis (1989)

(3) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993)

Hazardous Substances Data Bank (HSDB)

12.2.5 Environmental Biodegradation

The test concentration of succinonitrile at 500 ppm was found to be toxic to microorganisms in sludges from 3 municipal treatment plants and inhibited biodegradation as determined using Warburg constant-volume respirometers(1). Succinonitrile (500 mg/L) reached 1.5, 2.4, and 3.8% of the theoretical **oxygen** demand after 6, 12, and 24 hours in a study using a Warburg respirometer and activated sludge solids (2,500 mg/L)(2). A mixed microbial culture isolated from an environment contaminated with organic cyanides and polychlorinated biphenyls was found to utilize nitriles, including succinonitrile, as growth substrates(3).

Aeromonas sp. BN 7013 was isolated from a soil sample and was found to utilize succinonitrile as a sole source of **nitrogen**(4). A variant yeast strain, Candida famata, isolated from **gold** mine effluent was able to grow on various nitrile compounds, including succinonitrile, as a sole source of **nitrogen**, after acclimatization(5). Pseudomonas putida, a bacterium isolated from soil that can utilize high concentrations of **acetonitrile** as a sole source of **carbon** and **nitrogen**, could also utilize various nitriles, including succinonitrile(6).

(1) Lutin PA; J Water Pollut Control Fed 42: 1632-1642 (1970)

(2) Malaney GW, Gerhold RM; J Water Pollut Control Fed 4: R18-R33 (1969)

(3) Chapatwala KD et al; Environ Toxicol Chem 11: 1145-51 (1992)

(4) Kuwahara M et al; Hakkokogaku Kaishi 58: 441-8 (1980)

(5) Linardi VR et al; FEMS Microbiol Lett 144: 67-71 (1996)

(6) Nawaz MS et al; Appl Environ Microbiol 55: 2267-74 (1989)

- **Hazardous Substances Data Bank (HSDB)**

12.2.6 Environmental Abiotic Degradation

The rate constant for the vapor-phase reaction of succinonitrile with photochemically-produced hydroxyl radicals has been estimated as 4.3X10-14 cu cm/molecule-sec at 25 °C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 380 days at an atmospheric concentration of 5X10+5 hydroxyl radicals per cu cm(1). Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions(2). Succinonitrile is not expected to be susceptible to direct photolysis by sunlight, since it does not contain functional groups that are expected to absorb light with wavelengths >290 nm(SRC).

(1) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993)

(2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 7-4, 7-5 (1990)

- **Hazardous Substances Data Bank (HSDB)**

12.2.7 Environmental Bioconcentration

An estimated BCF of 3 was calculated for succinonitrile(SRC), using a log Kow of -0.99(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

(1) Tanii H, Hashimoto K; Arch Toxicol 57: 88-93 (1985)

(2) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999)

(3) Franke C et al; Chemosphere 29: 1501-14 (1994)

- **Hazardous Substances Data Bank (HSDB)**

12.2.8 Soil Adsorption / Mobility

Using a structure estimation method based on molecular connectivity indices(1), the Koc for succinonitrile can be estimated to be 28(SRC). According to a classification scheme(2), this estimated Koc value suggests that succinonitrile is expected to have very high mobility in soil.

(1) Meylan WM et al; Environ Sci Technol 26: 1560-67 (1992)

(2) Swann RL et al; Res Rev 85: 17-28 (1983)

- **Hazardous Substances Data Bank (HSDB)**

12.2.9 Volatilization from Water / Soil

The Henry's Law constant for succinonitrile is estimated as 6.5X10-9 atm-cu m/mole(SRC) derived from its vapor pressure, 0.00778 mm Hg(1), and water solubility, 126.9 g/L(2). This Henry's Law constant indicates that succinonitrile is expected to be essentially nonvolatile from water surfaces(3). Succinonitrile's estimated Henry's Law constant indicates that volatilization from moist soil surfaces is not expected to occur(SRC). Succinonitrile is not expected to volatilize from dry soil surfaces(SRC) based upon its vapor pressure(1).

(1) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, DC: Taylor and Francis (1989)

(2) Yalkowsky SH, He Y, eds; Handbook of Aqueous Solubility Data. Boca Raton, FL: CRC Press LLC, p. 82 (2003)

(3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990)

- **Hazardous Substances Data Bank (HSDB)**

12.2.10 Probable Routes of Human Exposure

NIOSH (NOES Survey 1981-1983) has statistically estimated that 1,440 workers are potentially exposed to succinonitrile in the US(1). Occupational exposure to succinonitrile may occur through inhalation and dermal contact with this compound at workplaces where succinonitrile is produced or used(SRC).

(1) NIOSH; National Occupational Exposure Survey (NOES) (1983)

- Hazardous Substances Data Bank (HSDB)

13 Literature

13.1 Consolidated References

- PubChem

13.2 NLM Curated PubMed Citations

PubChem

13.3 Springer Nature References

Springer Nature

13.4 Thieme References

Thieme Chemistry

13.5 Wiley References

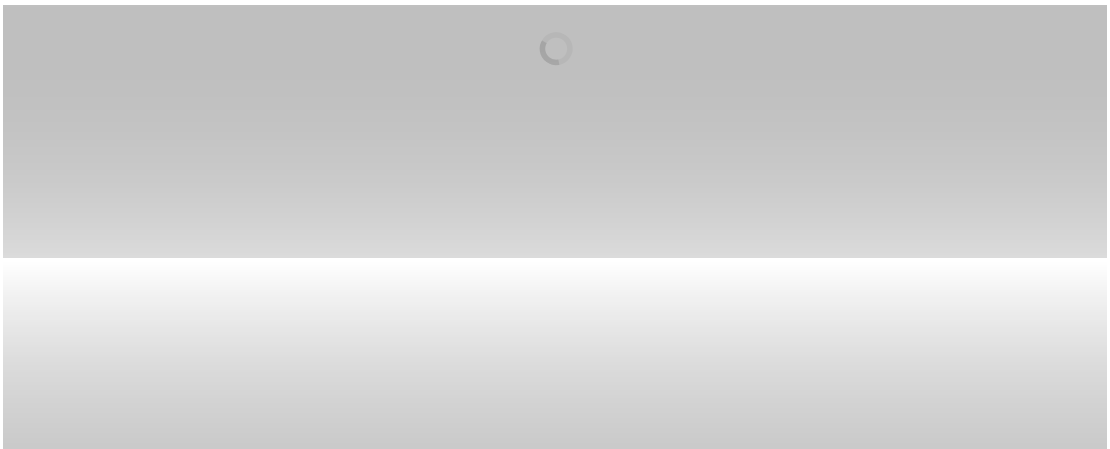
- Wiley

13.6 Nature Journal References

Patel et al. Common origins of RNA, protein and lipid precursors in a cyanosulfidic protometabolism. Nature Chemistry, doi: 10.1038/nchem.2202, published online 16 March 2015 http://www.nature.com/nchem

- Nature Chemistry

13.7 Chemical Co-Occurrences in Literature



PubChem

13.8 Chemical-Gene Co-Occurrences in Literature

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13.9 Chemical-Disease Co-Occurrences in Literature

PubChem

14 Patents

14.1 Depositor-Supplied Patent Identifiers

PubChem

Link to all deposited patent identifiers

PubChem

14.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=IAHFWCOBPZCAEA-UHFFFAOYSA-N

PATENTSCOPE (WIPO)

14.3 Chemical Co-Occurrences in Patents

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14.4 Chemical-Disease Co-Occurrences in Patents

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14.5 Chemical-Gene Co-Occurrences in Patents

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17.2 ChemIDplus

ChemIDplus

17.3 CAMEO Chemicals

CAMEO Chemicals

17.4 UN GHS Classification

GHS Classification (UNECE)

17.5 EPA CPDat Classification

EPA Chemical and Products Database (CPDat)

17.6 NORMAN Suspect List Exchange Classification

- NORMAN Suspect List Exchange

17.7 EPA DSSTox Classification

- EPA DSSTox

17.8 EPA TSCA and CDR Classification

- EPA Chemicals under the TSCA

17.9 EPA Substance Registry Services Tree

EPA Substance Registry Services

18 Information Sources

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Succinonitrile

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Succinonitrile (EC: 203-783-9)

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EPA CPDat Classification

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Succinonitrile

http://www.hmdb.ca/metabolites/HMDB0258544

HMDB0258544_nmr_one_2144

https://hmdb.ca/metabolites/HMDB0258544#spectra

22. SpectraBase

succinonitrile

https://spectrabase.com/spectrum/JHzyJkHU2VH

Succinonitrile

https://spectrabase.com/spectrum/HIw2A6n337V

SUCCINONITRILE

https://spectrabase.com/spectrum/EU2aKA5QAye

Butanodinitrile

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BUTANEDINITRILE

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Butanedinitrile

https://spectrabase.com/spectrum/12fQSI4mTwL

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https://spectrabase.com/spectrum/LE91OKc3mS7

Succinonitrile

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https://spectrabase.com/spectrum/3RgWz2WxTnX

Succinonitrile

https://spectrabase.com/spectrum/GEwRd7l9JI6

Succinonitrile

https://spectrabase.com/spectrum/Gf34jPUpuCp

Butanodinitrile

https://spectrabase.com/spectrum/LdEarZCo7q5

Butanodinitrile

https://spectrabase.com/spectrum/GIsD8uhAPFN

23. Japan Chemical Substance Dictionary (Nikkaji)

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query=exists(compound.metaData.name:%27InChIKey%27%20and%20compound.metaData.value:%27IAHFWCOBPZCAEA-UHFFFAOYSA-N%27)

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27. Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=6037506-42671363

28. SpringerMaterials

1,2-dicyanoethane

https://materials.springer.com/substanceprofile/docs/smsid_bltsssaowxuvidsr

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33. Wiley

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34. PubChem

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35. Medical Subject Headings (MeSH)

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MeSH Tree

http://www.nlm.nih.gov/mesh/meshhome.html

36. GHS Classification (UNECE)

GHS Classification Tree

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37. NORMAN Suspect List Exchange

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EPA SRS List Classification
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39. PATENTSCOPE (WIPO)

SID 403031316
https://pubchem.ncbi.nlm.nih.gov/substance/403031316

PubChem

COMPOUND SUMMARY

1,2-Bis(2-cyanoethoxy)ethane

PubChem CID	76921
Structure	2D 3D
Chemical Safety	Flammable Corrosive Acute Toxic Irritant Health Hazard Environmental Hazard Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_8H_{12}N_2O_2$
Synonyms	3386-87-6 1,2-Bis(2-cyanoethoxy)ethane Ethylene glycol bis(propionitrile) ether 3,3'-(Ethylenedioxy)dipropionitrile 3,3'-(Ethylenedioxy)dipropiononitrile View More...
Molecular Weight	168.19 g/mol *Computed by PubChem 2.2 (PubChem release 2021.10.14)*

Dates	Create:	Modify:
	2005-03-26	2024-12-14

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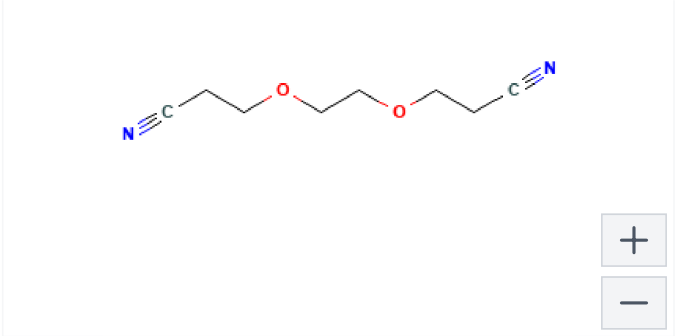
1 Structures

1.1 2D Structure

Chemical Structure Depiction



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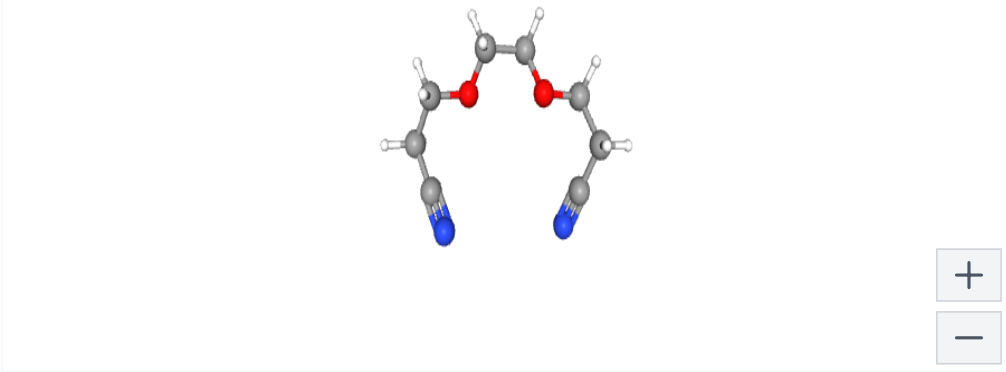
1.2 3D Conformer

Interactive Chemical Structure Model

Ball and Stick Sticks Wire-Frame Space-Filling

Show Hydrogens Animate



First Previous Conformer 1 of 10 Next Last

PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

3-[2-(2-cyanoethoxy)ethoxy]propanenitrile

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

PubChem

2.1.2 InChI

InChI=1S/C8H12N2O2/c9-3-1-5-11-7-8-12-6-2-4-10/h1-2,5-8H2

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2.1.3 InChIKey

VTHRQKSLPFJQHN-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

PubChem

2.1.4 SMILES

C(COCCOCCC#N)C#N

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PubChem

2.2 Molecular Formula

$C_8H_{12}N_2O_2$

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2.3 Other Identifiers

2.3.1 CAS

3386-87-6

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2.3.2 European Community (EC) Number

222-208-2

- European Chemicals Agency (ECHA)

2.3.3 UNII

233IZ4495B

- FDA Global Substance Registration System (GSRS)

2.3.4 ChEMBL ID

CHEMBL3182354

- ChEMBL

2.3.5 DSSTox Substance ID

DTXSID0044656

- EPA DSSTox

2.3.6 Nikkaji Number

J150.755I

- Japan Chemical Substance Dictionary (Nikkaji)

2.3.7 NSC Number

69063

- DTP/NCI

2.3.8 Wikidata

Q27253708

- Wikidata

2.4 Synonyms

2.4.1 Depositor-Supplied Synonyms

3386-87-6	3,3'-(ethane-1,2-diylbis(oxy))dipropanenitrile	Ethyle
1,2-Bis(2-cyanoethoxy)ethane	1,2-Bis(beta-cyanoethoxyethane)	Ethyle
Ethylene glycol bis(propionitrile) ether	MFCD00019871	3,3'-[
3,3'-(Ethylenedioxy)dipropionitrile	NSC 69063	UNII-
3,3'-(Ethylenedioxy)dipropiononitrile	Propionitrile, 3,3'-(ethylenedioxy)di-	1,2-Bi
3-[2-(2-Cyanoethoxy)ethoxy]propanenitrile	DTXSID0044656	EINEC
ETHYLENEGLYCOLBIS(PROPIONITRILE)ETHER	NSC-69063	Ethyle
Ethylene glycol bis(cyanoethyl) ether	Propanenitrile, 3,3'-(1,2-ethanediylbis(oxy))bis-	AI3-0
Ethylene glycol bis(2-cyanoethyl) ether	1,2-Bis(.beta.-cyanoethyloxy)ethane	4,7-d
Propanenitrile, 3,3'-[1,2-ethanediylbis(oxy)]bis-	233IZ4495B	SCHE

- PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference

Molecular Weight	168.19 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
XLogP3-AA	-0.7	Computed by XLogP3 3.0 (PubChem release 2021.10.14)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Hydrogen Bond Acceptor Count	4	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Rotatable Bond Count	7	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Exact Mass	168.089877630 Da	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Monoisotopic Mass	168.089877630 Da	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Topological Polar Surface Area	66$Å^2$	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Heavy Atom Count	12	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	164	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.10.14)

- PubChem

3.2 SpringerMaterials Properties

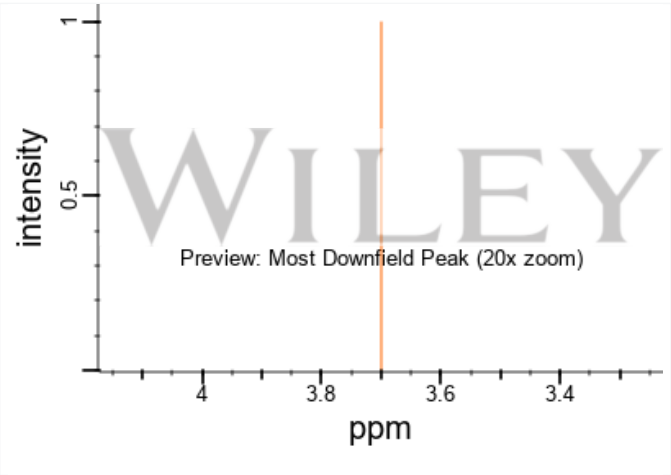
Viscosity

- SpringerMaterials

4 Spectral Information

4.1 1D NMR Spectra

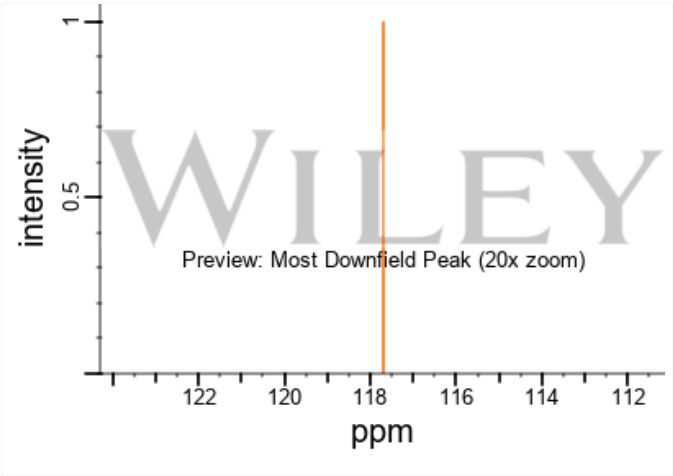
4.1.1 1H NMR Spectra

Instrument Name	Varian CFT-20
Copyright	Copyright © 2009-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

- SpectraBase

4.1.2 13C NMR Spectra

Instrument Name	Bruker AC-250

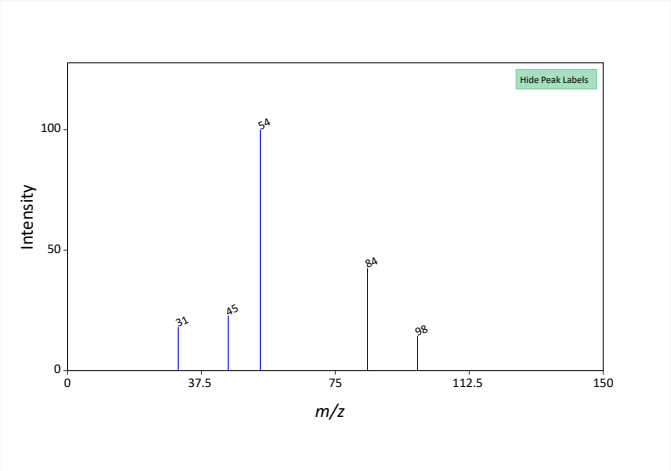
Copyright	Copyright © 2002-2024 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
Thumbnail	

SpectraBase

4.2 Mass Spectrometry

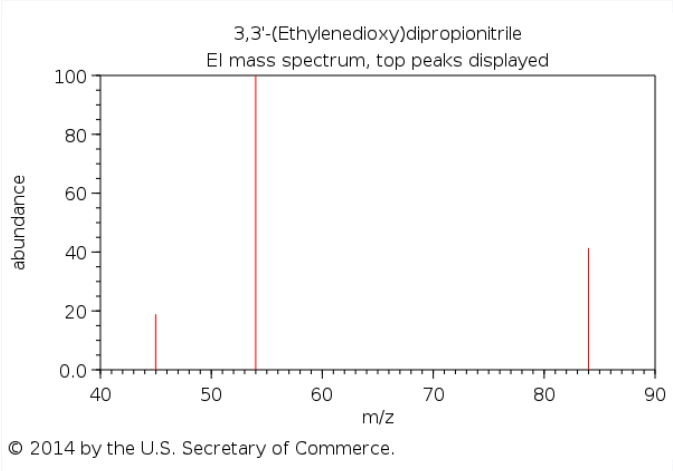
4.2.1 GC-MS

1 of 6	View All
MoNA ID	JP006773
MS Category	Experimental
MS Type	GC-MS
MS Level	MS1
Instrument	HITACHI RMU-6M
Instrument Type	EI-B
Ionization Mode	positive

Top 5 Peaks	54 99.99 84 42.52 45 22.79 31 18.03 98 14.29
SPLASH	splash10-0ue9-9000000000-8e7dde93da89b12df68d
Thumbnail	
License	CC BY-NC-SA

MassBank of North America (MoNA)

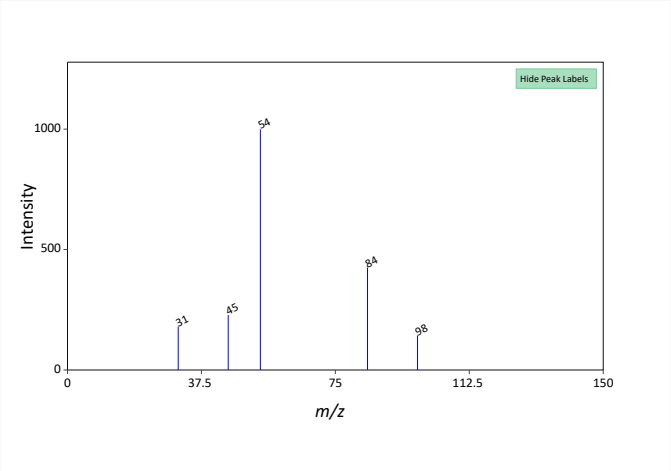
2 of 6	View All
NIST Number	233574
Library	Main library
Total Peaks	65
m/z Top Peak	54
m/z 2nd Highest	84
m/z 3rd Highest	45

Thumbnail	

NIST Mass Spectrometry Data Center

4.2.2 Other MS

Accession ID	MSBNK-Fac_Eng_Univ_Tokyo-JP006773
Authors	YAMAMOTO M, DEP. CHEMISTRY, FAC. SCIENCE, NARA WOMEN'S UNIV.
Instrument	HITACHI RMU-6M
Instrument Type	EI-B
MS Level	MS
Ionization Mode	POSITIVE
Ionization	ENERGY 70 eV
Top 5 Peaks	54 999 84 425 45 228 31 180 98 143
SPLASH	splash10-0ue9-9000000000-8e7dde93da89b12df68d

Thumbnail	
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MassBank Europe

5 Related Records

5.1 Related Compounds with Annotation

Follow these links to do a live 2D search or do a live 3D search for this compound, sorted by annotation score. This section is deprecated (see here for details), but these live search links provide equivalent functionality to the table that was previously shown here.

PubChem

5.2 Related Compounds

Same Parent, Exact Count	5
Mixtures, Components, and Neutralized Forms Count	13
Similar Compounds (2D)	View in PubChem Search
Similar Conformers (3D)	View in PubChem Search

PubChem

5.3 Substances

5.3.1 Related Substances

All Count	119
Same Count	102
Mixture Count	17

PubChem

5.3.2 Substances by Category

PubChem

6 Chemical Vendors

- PubChem

7 Use and Manufacturing

7.1 General Manufacturing Information

EPA TSCA Commercial Activity Status

Propanenitrile, 3,3'-[1,2-ethanediylbis(oxy)]bis-: ACTIVE

- EPA Chemicals under the TSCA

8 Safety and Hazards

8.1 Hazards Identification

8.1.1 GHS Classification

Pictogram(s)	Flammable, Corrosive, Acute Toxic, Irritant, Health Hazard, Environmental Hazard
Signal	Danger
GHS Hazard Statements	H225 (45%): Highly Flammable liquid and vapor [**Danger** Flammable liquids] H301 (55%): Toxic if swallowed [**Danger** Acute toxicity, oral] H311 (45%): Toxic in contact with skin [**Danger** Acute toxicity, dermal]

	H314 (45%): Causes severe skin burns and eye damage [**Danger** Skin corrosion/irritation] H315 (55%): Causes skin irritation [**Warning** Skin corrosion/irritation] H317 (45%): May cause an allergic skin reaction [**Warning** Sensitization, Skin] H318 (45%): Causes serious eye damage [**Danger** Serious eye damage/eye irritation] H319 (55%): Causes serious eye irritation [**Warning** Serious eye damage/eye irritation] H331 (45%): Toxic if inhaled [**Danger** Acute toxicity, inhalation] H335 (50%): May cause respiratory irritation [**Warning** Specific target organ toxicity, single exposure; Respiratory tract irritation] H350 (45%): May cause cancer [**Danger** Carcinogenicity] H411 (45%): Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]
Precautionary Statement Codes	P203, P210, P233, P240, P241, P242, P243, P260, P261, P262, P264, P264+P265, P270, P271, P272, P273, P280, P301+P316, P301+P330+P331, P302+P352, P302+P361+P354, P303+P361+P353, P304+P340, P305+P351+P338, P305+P354+P338, P316, P317, P318, P319, P321, P330, P332+P317, P333+P317, P337+P317, P361+P364, P362+P364, P363, P370+P378, P391, P403+P233, P403+P235, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided per 20 reports by companies from 4 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

- European Chemicals Agency (ECHA)

8.1.2 Hazard Classes and Categories

Flam. Liq. 2 (45%)

Acute Tox. 3 (55%)

Acute Tox. 3 (45%)

Skin Corr. 1C (45%)

Skin Irrit. 2 (55%)

Skin Sens. 1 (45%)

Eye Dam. 1 (45%)

Eye Irrit. 2A (55%)

Acute Tox. 3 (45%)

STOT SE 3 (50%)

Carc. 1B (45%)

Aquatic Chronic 2 (45%)

- European Chemicals Agency (ECHA)

9 Literature

9.1 Consolidated References

- PubChem

9.2 Springer Nature References

Springer Nature

9.3 Chemical Co-Occurrences in Literature

PubChem

10 Patents

10.1 Depositor-Supplied Patent Identifiers

- PubChem

Link to all deposited patent identifiers

- PubChem

10.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=VTHRQKSLPFJQHN-UHFFFAOYSA-N

- PATENTSCOPE (WIPO)

10.3 Chemical Co-Occurrences in Patents

- PubChem

10.4 Chemical-Disease Co-Occurrences in Patents

PubChem

11 Biological Test Results

11.1 BioAssay Results

PubChem

12 Classification

12.1 ChemIDplus

ChemIDplus

12.2 UN GHS Classification

GHS Classification (UNECE)

12.3 NORMAN Suspect List Exchange Classification

NORMAN Suspect List Exchange

12.4 EPA DSSTox Classification

EPA DSSTox

12.5 EPA TSCA and CDR Classification

EPA Chemicals under the TSCA

12.6 EPA Substance Registry Services Tree

EPA Substance Registry Services

12.7 MolGenie Organic Chemistry Ontology

MolGenie

13 Information Sources

FILTER BY SOURCE

ALL SOURCES

1. **CAS Common Chemistry**

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3,3'-[1,2-Ethanediylbis(oxy)]bis[propanenitrile]

https://commonchemistry.cas.org/detail?cas_rn=3386-87-6

2. **ChemIDplus**

LICENSE
https://www.nlm.nih.gov/copyright.html

3,3'-(Ethylenedioxy)dipropiononitrile

https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0003386876

ChemIDplus Chemical Information Classification

https://pubchem.ncbi.nlm.nih.gov/source/ChemIDplus

3. **DTP/NCI**

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https://www.cancer.gov/policies/copyright-reuse

1,2-Bis(2-cyanoethoxy)ethane

https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=69063

4. **EPA Chemicals under the TSCA**

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https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

Propanenitrile, 3,3'-[1,2-ethanediylbis(oxy)]bis-

https://www.epa.gov/chemicals-under-tsca

EPA TSCA Classification

https://www.epa.gov/tsca-inventory

5. EPA DSSTox

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

3,3'-(Ethylenedioxy)dipropiononitrile

https://comptox.epa.gov/dashboard/DTXSID0044656

CompTox Chemicals Dashboard Chemical Lists

https://comptox.epa.gov/dashboard/chemical-lists/

6. European Chemicals Agency (ECHA)

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https://echa.europa.eu/web/guest/legal-notice

3,3'-(ethylenedioxy)dipropiononitrile

https://echa.europa.eu/substance-information/-/substanceinfo/100.020.190

3,3'-(ethylenedioxy)dipropiononitrile (EC: 222-208-2)

https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/118898

7. FDA Global Substance Registration System (GSRS)

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https://www.fda.gov/about-fda/about-website/website-policies#linking

3,3'-(ETHYLENEDIOXY)DIPROPIONONITRILE

https://gsrs.ncats.nih.gov/ginas/app/beta/substances/233IZ4495B

8. ChEMBL

LICENSE
Access to the web interface of ChEMBL is made under the EBI's Terms of Use (http://www.ebi.ac.uk/Information/termsofuse.html). The ChEMBL data is made available on a Creative Commons Attribution-Share Alike 3.0 Unported License (http://creativecommons.org/licenses/by-sa/3.0/).

http://www.ebi.ac.uk/Information/termsofuse.html

https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL3182354/

9. ## Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J150.755I

10. ## MassBank Europe

LICENSE
https://github.com/MassBank/MassBank-web/blob/main/MassBank-Project/LICENSE.txt

ETHYLENE GLYCOL BIS(PROPIONITRILE) ETHER
https://massbank.eu/MassBank/Result.jsp?inchikey=VTHRQKSLPFJQHN-UHFFFAOYSA-N

11. ## MassBank of North America (MoNA)

LICENSE
The content of the MoNA database is licensed under CC BY 4.0.
https://mona.fiehnlab.ucdavis.edu/documentation/license

ETHYLENE GLYCOL BIS(PROPIONITRILE) ETHER
https://mona.fiehnlab.ucdavis.edu/spectra/browse?query=exists(compound.metaData.name:%27InChIKey%27%20and%20compound.metaData.value:%27VTHRQKSLPFJQHN-UHFFFAOYSA-N%27)

12. ## NIST Mass Spectrometry Data Center

LICENSE
Data covered by the Standard Reference Data Act of 1968 as amended.
https://www.nist.gov/srd/public-law

3,3'-(Ethylenedioxy)dipropionitrile
http://www.nist.gov/srd/nist1a.cfm

13. ## SpectraBase

PROPANENITRILE, 3,3'-[1,2-ETHANEDIYLBIS(OXY)]BIS-
https://spectrabase.com/spectrum/ZTWuRVabGO

PROPANENITRILE, 3,3'-[1,2-ETHANEDIYLBIS(OXY)]BIS-
https://spectrabase.com/spectrum/Ddnr3mkmbqH

3,3'-(ethylenedioxy)dipropionitrile
https://spectrabase.com/spectrum/zAHTE5s7x8

1,8-Dicyano-3,6-dioxa-octane
https://spectrabase.com/spectrum/G57QNt1CWT2

14. ## Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=12042340-123749534

15. ## SpringerMaterials

4,7-dioxa-decanedinitrile

https://materials.springer.com/substanceprofile/docs/smsid_kmkdmwveexmkjucv

16. ## Wikidata

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3,3'-(ethylenedioxy)dipropiononitrile

https://www.wikidata.org/wiki/Q27253708

17. PubChem

https://pubchem.ncbi.nlm.nih.gov

18. ## GHS Classification (UNECE)

GHS Classification Tree

http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

19. ## NORMAN Suspect List Exchange

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Data: CC-BY 4.0; Code (hosted by ECI, LCSB): Artistic-2.0
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NORMAN Suspect List Exchange Classification

https://www.norman-network.com/nds/SLE/

20. ## EPA Substance Registry Services

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https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

EPA SRS List Classification

https://sor.epa.gov/sor_internet/registry/substreg/LandingPage.do

21. ## MolGenie

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MolGenie Organic Chemistry Ontology

https://github.com/MolGenie/ontology/

22. ## PATENTSCOPE (WIPO)

SID 403401166

https://pubchem.ncbi.nlm.nih.gov/substance/403401166