

COMPOUND

Adiponitrile

Cite

Download

PubChem CID

8128

Structure



2D



3D



Crystal

Primary Hazards



Acute Toxic



Irritant

[Laboratory Chemical Safety Summary \(LCSS\) Datasheet](#)

Molecular Formula

C₆H₈N₂
CN(CH₂)₄CN

Synonyms

ADIPONITRILE
Hexanedinitrile
1,4-Dicyanobutane
111-69-3
Adipodinitrile

[View More...](#)

Molecular Weight

108.14 g/mol

Computed by PubChem 2.2 (PubChem release 2025.09.15)

Dates

Create: 2005-03-26
Modify: 2026-06-13

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 an important precursor to the polymer [nylon 66](#). (L584)

► [Toxin and Toxin Target Database \(T3DB\)](#)

Contents

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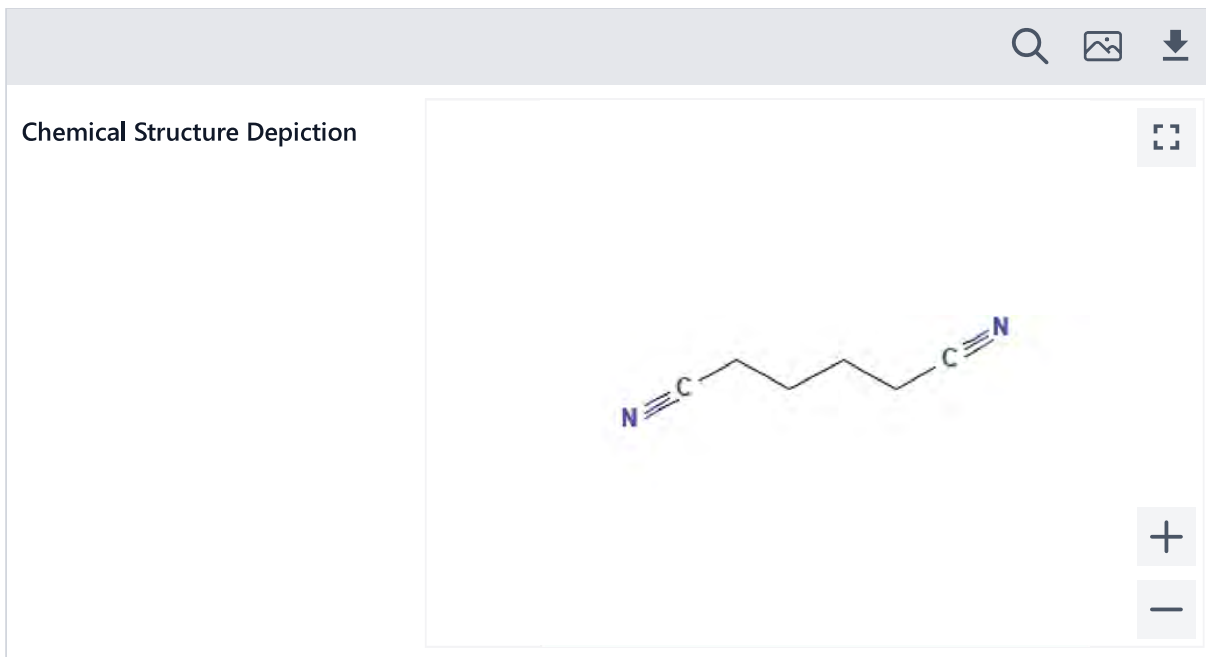
17 Classification

18 Information Sources

1 Structures



1.1 2D Structure



► PubChem

1.2 3D Conformer



[► PubChem](#)

1.3 Crystal Structures



1 of 2 items		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 2.9.3 (PubChem release 2025.09.15)

► [PubChem](#)

2.1.2 InChI



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

Computed by InChI 1.07.4 (PubChem release 2025.09.15)

► [PubChem](#)

2.1.3 InChIKey



BTGRAWJCKBQKAO-UHFFFAOYSA-N

Computed by InChI 1.07.4 (PubChem release 2025.09.15)

► [PubChem](#)

2.1.4 SMILES



C(CCC#N)CC#N

Computed by OEChem 4.2.0 (PubChem release 2025.09.15)

► [PubChem](#)

2.2 Molecular Formula



Computed by PubChem 2.2 (PubChem release 2025.09.15)

► [Australian Industrial Chemicals Introduction Scheme \(AICIS\)](#); [CAMEO Chemicals](#); [PAC Chemical D...](#)



► [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

- ▶ [CAMEO Chemicals; Emergency Response Guidebook \(ERG\); ILO-WHO International Chemical Safe...](#)

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



NSC7617

- ▶ 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	NSC 7617	UN2205
Hexanedinitrile	Adipinsaeuredinitril	MFCD00001975	BRN 1740005
1,4-Dicyanobutane	Hexanedioic acid, dinitrile	butane-1,4-dicarbonitrile	UNII-SYT33B89
111-69-3	DTXSID3021936	Nitrile adipico [Italian]	Adipic dinitrile
Adipodinitrile	SYT33B89II	Adipinsaeuredinitril [German]	AI3-11080
Adipylidinitrile	NSC-7617	CAS-111-69-3	EINECS 270-153
Adipic acid dinitrile	DTXCID201936	CCRIS 4570	Adiponitrile, 99
Nitrile adipico	adiponitril	HSDB 627	hexane-1,6-dini
Tetramethylene dicyanide	RefChem:915174	EINECS 203-896-3	ADIPONITRILE
Tetramethylene cyanide	203-896-3	Hexanedioic acid dinitrile	BUTANEDICARI

► [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 2025.09.15)
XLogP3	-0.3	Computed by XLogP3 3.0 (PubChem release 2025.09.15)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Hydrogen Bond Acceptor Count	2	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Rotatable Bond Count	3	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Exact Mass	108.068748264 Da	Computed by PubChem 2.2 (PubChem release 2025.09.15)

Monoisotopic Mass	108.068748264 Da	Computed by PubChem 2.2 (PubChem release 2025.09.15)
Topological Polar Surface Area	47.6 Å ²	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Heavy Atom Count	8	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	113	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
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 2025.09.15)

► [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; CBI

► [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

Hide, 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...](#)

295 °C @760 [mm Hg]

► [PAC Chemical Database, U.S. Department of Energy](#)

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...](#)

2 °C

► [PAC Chemical Database, U.S. Department of Energy](#)

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...**

0.963 @ 20°C

► **PAC Chemical Database, U.S. Department of Energy**

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...](#)

0.001 [mm Hg] @20 °C

► [PAC Chemical Database, U.S. Department of Energy](#)

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

► SpringerMaterials

3.4 Chemical Classes



Nitrogen Compounds -> Nitriles

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

Flammable agents - 2nd degree

Reactive agents - 1st degree

► NJDOH RTK Hazardous Substance List

3.4.1 Pesticides



Pesticide -> EPA IRIS

► EPA Integrated Risk Information System (IRIS)

4 Spectral Information



4.1 1D NMR Spectra



1 of 2 items

1D NMR Spectra

¹H NMR: SAD 6702 (Sadtler Research Laboratories spectral collection)

► [Hazardous Substances Data Bank \(HSDB\)](#)

2 of 2 items

1D NMR Spectra

[NMRShiftDB Link](#)

► [NMRShiftDB](#)

4.1.1 ¹H NMR Spectra



1 of 2 items

Spectra ID [2155](#)

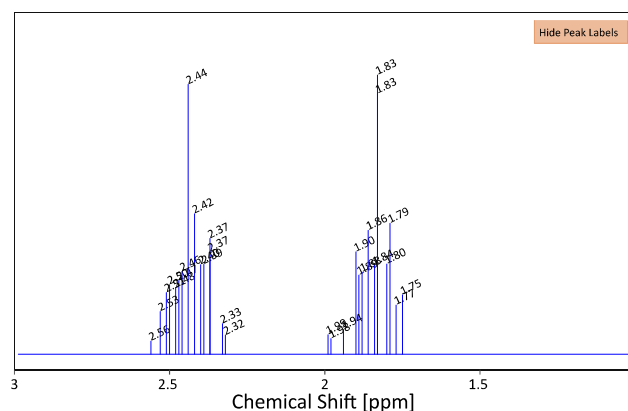
Instrument Type JEOL

Frequency 90 MHz

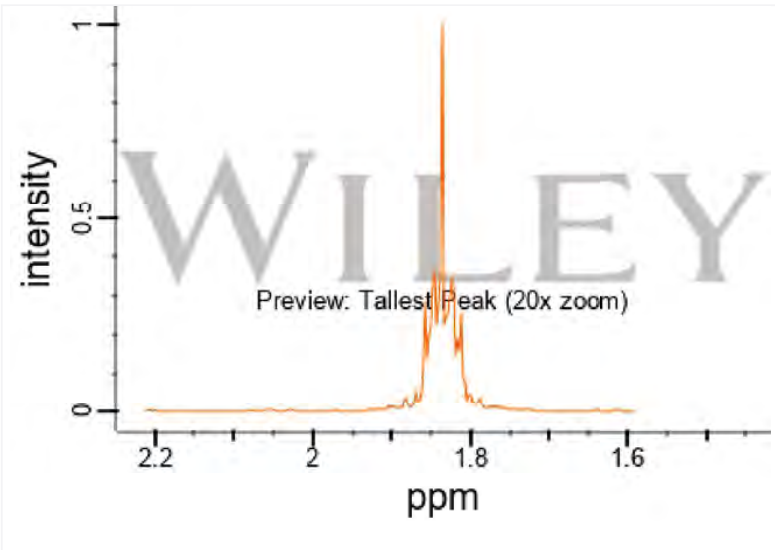
Solvent CDCl₃

Shifts [ppm]:Intensity 2.48:238.00, 2.53:153.00, 2.42:503.00, 2.37:414.00, 1.89:283.00, 1.90:366.00, 2.39:322.00, 1.83:1000.00, 1.75:212.00, 2.56:47.00, 2.37:366.00, 2.50:249.00, 1.88:294.00, 1.80:323.00, 1.94:88.00, 2.32:68.00, 1.77:176.00, 1.86:444.00, 1.79:469.00, 2.47:263.00, 1.84:318.00, 2.33:109.00, 1.83:933.00, 1.98:56.00, 2.40:321.00, 2.44:966.00, 1.99:70.00, 2.46:296.00, 2.51:221.00

Thumbnail



► [Human Metabolome Database \(HMDB\)](#)

2 of 2 items	
Instrument Name	BRUKER AC-300
Source of Sample	Tokyo Kasei Kogyo Company, Ltd., Tokyo, Japan
Copyright	Copyright © 1991-2025 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

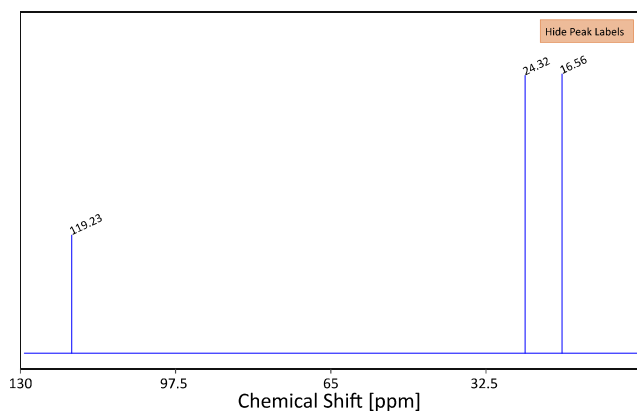
► [SpectraBase](#)

4.1.2 ¹³C NMR Spectra



1 of 2 items	
Spectra ID	2842
Instrument Type	Varian
Frequency	25.16 MHz
Solvent	CDCl ₃
Shifts [ppm]:Intensity	16.56:1000.00, 24.32:995.00, 119.23:423.00

Thumbnail



► [Human Metabolome Database \(HMDB\)](#)

2 of 2 items

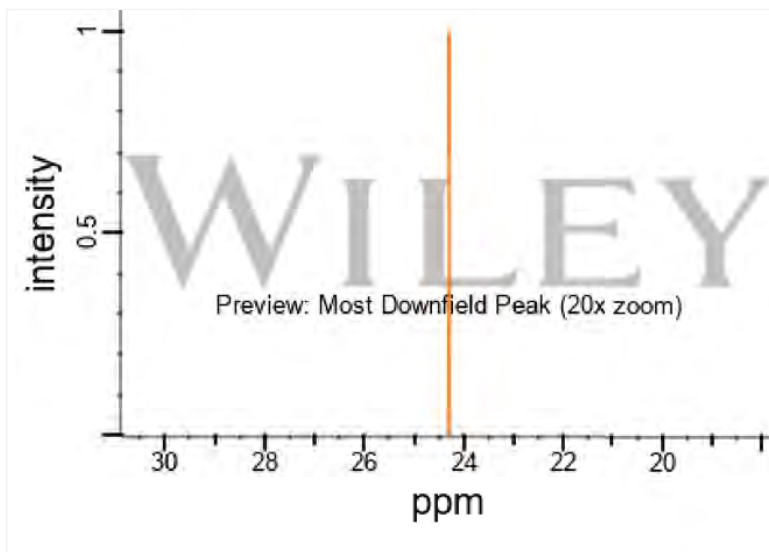
Source of Sample

Tokyo Kasei Kogyo Company, Ltd., Tokyo, Japan

Copyright

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Thumbnail



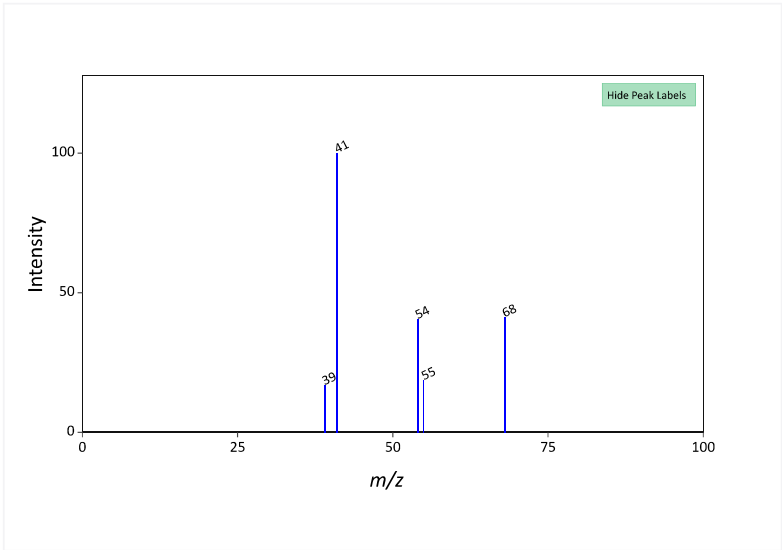
► [SpectraBase](#)

4.2 Mass Spectrometry

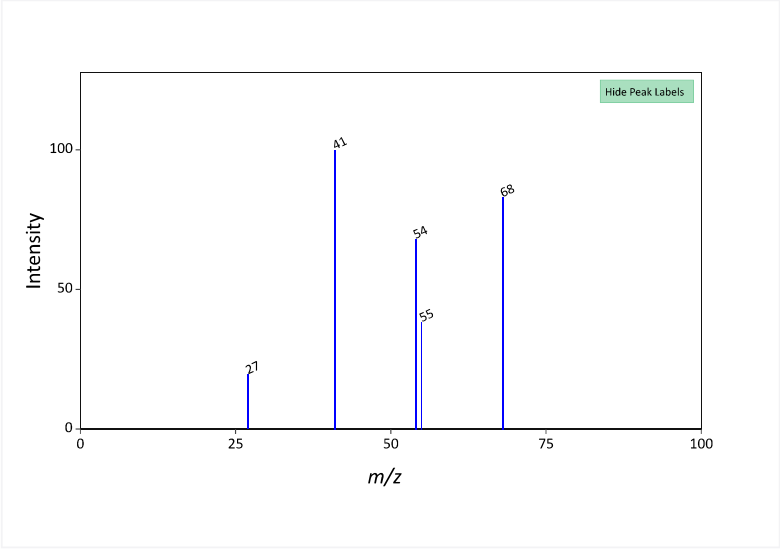


4.2.1 GC-MS



1 of 6 items		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 6 items		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	

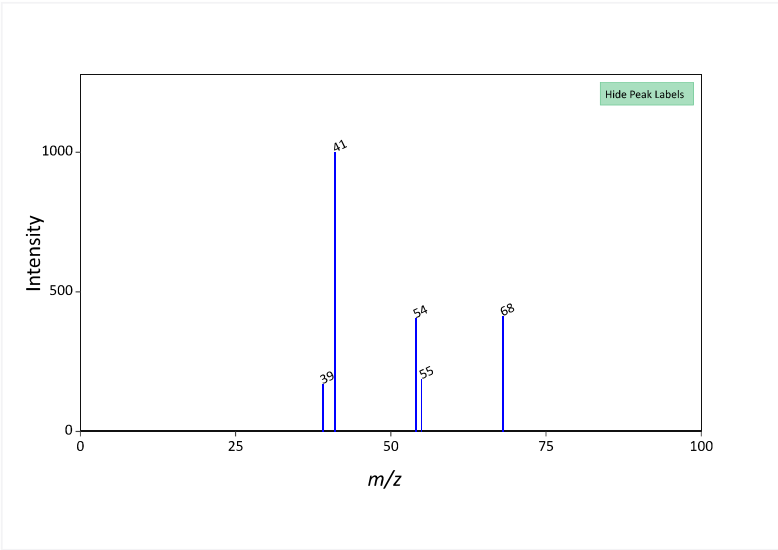
► [MassBank of North America \(MoNA\)](#)

4.2.2 Other MS



1 of 3 items		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 items		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	 Hide Peak Labels	

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



Instrument Name

Bruker IFS 85

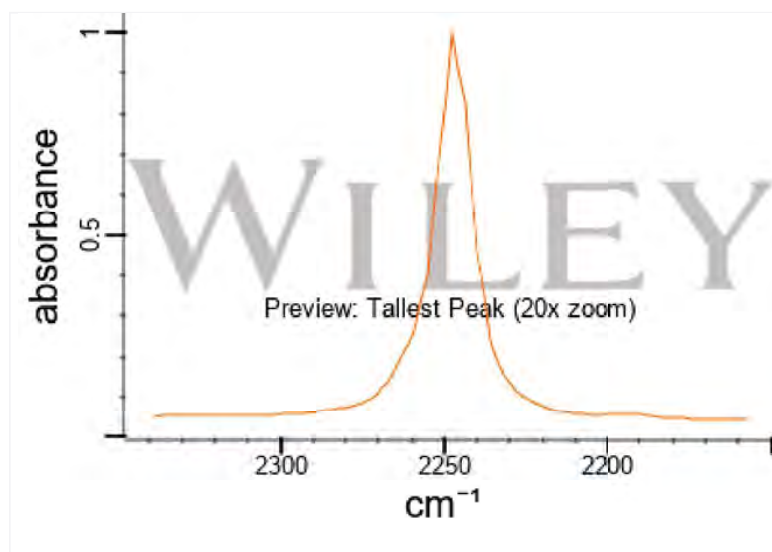
Technique

Cell

Copyright

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Thumbnail

[► SpectraBase](#)

4.3.2 ATR-IR Spectra



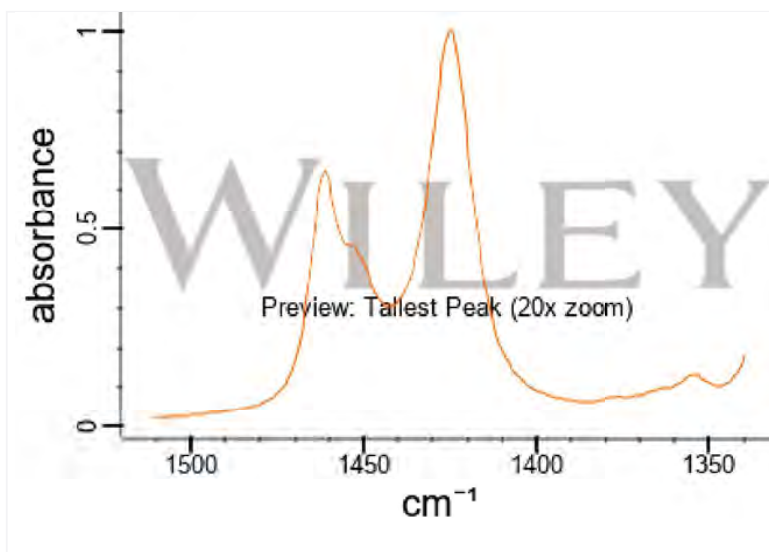
Technique

ATR-Cylindrical Internal Reflectance (CIR)

Copyright

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Thumbnail



► SpectraBase

4.3.3 Vapor Phase IR Spectra



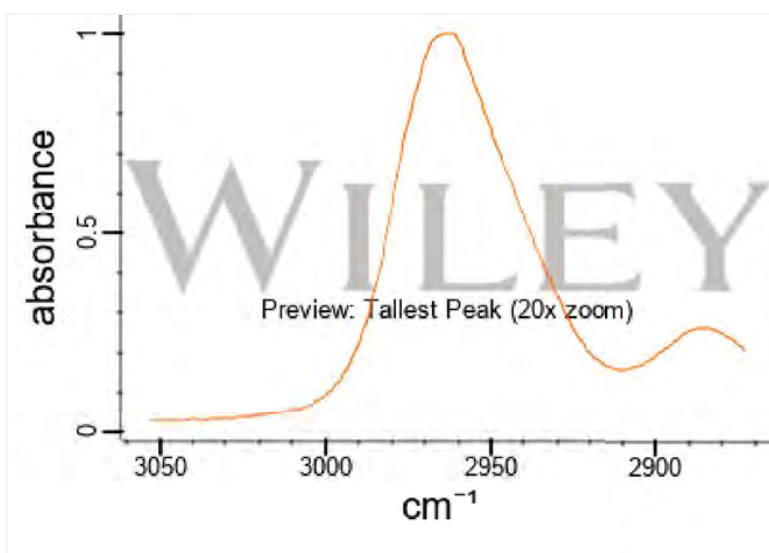
Technique

Vapor Phase

Copyright

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Thumbnail



► SpectraBase

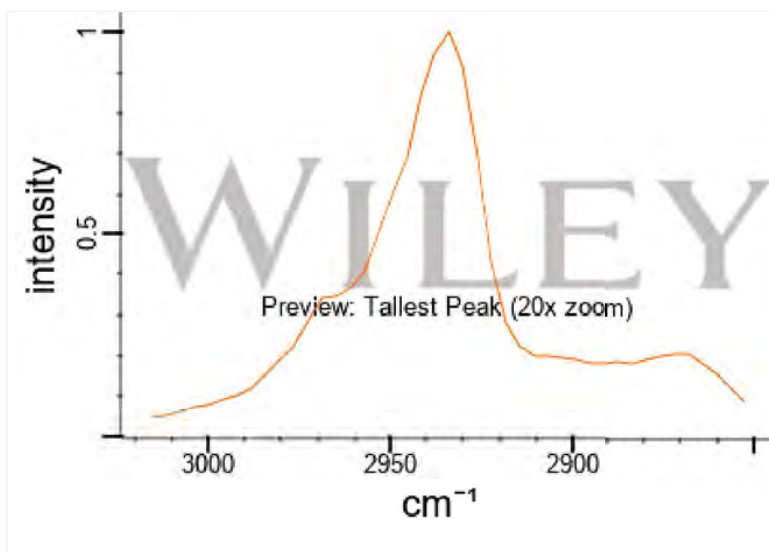
4.4 Raman Spectra



Copyright

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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 [the neighbor discontinuation help page](#) 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	4
Same Parent, Connectivity Count	27
Same Parent, Exact Count	24

Mixtures, Components, and Neutralized Forms Count	127
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



516561082

► [PubChem](#)

5.3.2 Related Substances



All Count	336
Same Count	168
Mixture Count	168

► [PubChem](#)

5.3.3 Substances by Category



► PubChem

5.4 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)

► 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)

► [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 Industry Uses



Other
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

2023: 1,000,000,000 - <2,500,000,000 lb

2022: 1,000,000,000 - <2,500,000,000 lb

2021: 1,000,000,000 - <2,500,000,000 lb

2020: 1,000,000,000 - <2,500,000,000 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 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



11.1.1 GHS Classification



1 of 3 items		View All
Pictogram(s)	 Acute Toxic Irritant	
Signal	<u>Danger</u>	
GHS Hazard Statements	H301 (100%): Toxic if swallowed <u>Danger</u> Acute toxicity, oral] H315 (18.3%): Causes skin irritation <u>Warning</u> Skin corrosion/irritation]	

	H319 (18.8%): Causes serious eye irritation [Warning Serious eye damage/eye irritation] H330 (18.8%): Fatal if inhaled [Danger Acute toxicity, inhalation] H332 (79.5%): Harmful if inhaled [Warning Acute toxicity, inhalation] H335 (18.3%): 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
ECHA C&L Notifications Summary	<i>Aggregated GHS information provided per 224 reports by companies from 7 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.</i> <i>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. For more detailed information, please visit ECHA C&L website.</i>

► [European Chemicals Agency \(ECHA\)](#)

11.1.2 Hazard Classes and Categories



Acute Tox. 3 (100%)

Skin Irrit. 2 (18.3%)

Eye Irrit. 2 (18.8%)

Acute Tox. 2 (18.8%)

Acute Tox. 4 (79.5%)

STOT SE 3 (18.3%)

► [European Chemicals Agency \(ECHA\)](#)

[View More...](#)

11.1.3 NFPA Hazard Classification



1 of 2 items

[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 DOT Hazard Classification



Substance (Descriptions/Shipping Name)	Adiponitrile
DOT ID (UN/NA Number)	UN2205
Hazard Class/Label Code(s)	Div 6.1 Poisonous materials (49 eCFR § 173.132)
Packing Group	PG III: the degree of danger presented by the material is minor For more information about the packing group assignment, please visit 49 eCFR § 173
Placard/Label(s)	

► [US Code of Federal Regulations, Hazardous Materials, 49 CFR Part 172](#)

11.1.5 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](#)

ERG2024, 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 \(ERG\)](#)

11.1.6 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](#)

ERG2024, 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 \(ICSCs\)](#)

11.1.7 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](#)

11.1.8 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 \(HSDB\)](#)

11.1.9 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 Protective Action Criteria (PAC)



PAC-1

1.5 [ppm]

- ▶ [PAC Chemical Database, U.S. Department of Energy](#)

PAC-2

17 [ppm]

- ▶ [PAC Chemical Database, U.S. Department of Energy](#)

PAC-3

75 [ppm]

- ▶ [PAC Chemical Database, U.S. Department of Energy](#)

11.2.2 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: F.I.P. at or above 140 °F and below 200 °F.

- ▶ [The National Institute for Occupational Safety and Health \(NIOSH\)](#)

11.2.3 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...](#)

11.2.4 Upper Explosive Limit (UEL)



5 % (NIOSH, 2024)

- ▶ [CAMEO Chemicals](#)

5.0%

- ▶ [Occupational Safety and Health Administration \(OSHA\); The National Institute for Occupational S...](#)

11.2.5 Critical Temperature and 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 \(HSDB\)](#)

11.2.6 Explosive Limits and Potential



Explosive limits , vol% in air: 1.7-4.9

- ▶ [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

11.2.7 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](#)

ERG2024, 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 ingested or 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 continuous compressions. 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 \(ERG\)](#)

(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: ERG2024, 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: ERG2024, 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: ERG2024, 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 and 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: ERG2024, 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/m³)

► [Occupational Safety and Health Administration \(OSHA\)](#)

TWA 4 ppm (18 mg/m³)

► [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: ERG2024, 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 \(HSDB\)](#)

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 Fire Prevention



NO open flames.

- ▶ [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

11.7.12 Exposure Prevention



STRICT HYGIENE! IN ALL CASES CONSULT A DOCTOR!

- ▶ [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

11.7.13 Inhalation Prevention



Use ventilation, local exhaust or breathing protection.

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

11.7.14 Skin Prevention



Protective gloves. Protective clothing.

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

11.7.15 Eye Prevention



Wear face shield.

► [ILO-WHO International Chemical Safety Cards \(ICSCs\)](#)

11.7.16 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

► [Emergency Response Guidebook \(ERG\); The National Institute for Occupational Safety and Health...](#)

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 \(AICIS\)](#)

Hexanedinitrile is listed on the EPA's Chemical Data Reporting (CDR) system. Manufacturers and importers of **Hexanedinitrile** are required to report information about their production and use of this chemical to the EPA under the Toxic Substances Control Act (**TSCA**). (40 eCFR Part 711)

► [EPA Chemical Data Reporting \(CDR\)](#)

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 \(EPA\)](#)

New Jersey Worker and Community Right to Know Act

The New Jersey Worker and Community Right to Know Act requires public and private employers to provide information about hazardous substances at their workplaces. ([N.J.S.A. 34:5A-1 et. seq.](#))

► [NJDOH RTK Hazardous Substance List](#)

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)

► [Toxin and Toxin Target Database \(T3DB\)](#)

12.1.2 EPA IRIS Information



Substance	Adiponitrile
-----------	--------------

► [EPA Integrated Risk Information System \(IRIS\)](#)

12.1.3 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 \(HSDB\)](#)

12.1.4 Carcinogen Classification



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

► [Toxin and Toxin Target Database \(T3DB\)](#)

12.1.5 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)

► [Toxin and Toxin Target Database \(T3DB\)](#)

12.1.6 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)

► [Toxin and Toxin Target Database \(T3DB\)](#)

12.1.7 Signs and 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)

- ▶ [Toxin and Toxin Target Database \(T3DB\)](#)

12.1.8 Target Organs



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

- ▶ [The National Institute for Occupational Safety and Health \(NIOSH\)](#)

12.1.9 Adverse Effects



Other Poison - Chemical Asphyxiant

Dermatotoxin - Skin burns.

- ▶ [Haz-Map, Information on Hazardous Chemicals and Occupational Diseases](#)

12.1.10 Acute Effects



► [ChemIDplus](#)

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)

► [Toxin and Toxin Target Database \(T3DB\)](#)

12.1.12 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 \(HSDB\)](#)

12.1.13 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 \(HSDB\)](#)

12.1.14 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 \(HSDB\)](#)

12.1.15 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 \(HSDB\)](#)

12.2 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)

► [Toxin and Toxin Target Database \(T3DB\)](#)

12.2.1 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
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► [EPA Provisional Peer-Reviewed Toxicity Values \(PPRTVs\)](#)

12.2.2 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 \(RAIS\)](#)

12.2.3 NIOSH Toxicity Data



► [The National Institute for Occupational Safety and Health \(NIOSH\)](#)

12.2.4 Non-Human Toxicity Values



LD50 Guinea pig sc 50 mg/kg

Verschuereen, 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 \(HSDB\)](#)

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12.3 Ecological Information



12.3.1 Ecotoxicity Values



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

Verschuereen, 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 of bioassay not specified/

Verschuereen, 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/

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

► [Hazardous Substances Data Bank \(HSDB\)](#)

[View More...](#)

12.3.2 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 Dermal from Soil	0.1

► [EPA Regional Screening Levels for Chemical Contaminants at Superfund Sites](#)

12.3.3 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](#)

12.3.4 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 K_{oc} 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 K_{oc}. 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 \(HSDB\)](#)

12.3.5 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 \(HSDB\)](#)

12.3.6 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 \(HSDB\)](#)

12.3.7 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)**

12.3.8 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)**

12.3.9 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 \(HSDB\)](#)

12.3.10 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 \(HSDB\)](#)

12.3.11 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 \(HSDB\)](#)

12.3.12 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 \(HSDB\)](#)

12.3.13 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 \(HSDB\)](#)

12.3.14 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



► Medical Subject Headings (MeSH)

13.3 Springer Nature References



► Springer Nature

13.4 Thieme References



► Thieme Chemistry

13.5 Chemical Co-Occurrences in Literature



Showing 3 of 43 [View More](#) ▶ PubChem Showing 3 of 27 [View More](#) 

Disease	Selected evidence
---------	-------------------

Drug-Related Side Effects and Adverse Reactions	10 articles	View All 
	13-week inhalation toxicity study and fertility assessment in rats exposed to atmospheres containing adiponitrile PMID 2366257; DOI 10.1080/15287399009531423; Journal of Toxicology and Environmental Health 1990-07-01 Name matches: toxicity <i>adiponitrile</i> Health and Ecological Effects of Adiponitrile PMID 15198072; DOI 10.1081/dct-120030728; Drug and Chemical Toxicology 2004-04-22 (Review Article) Name matches: accidental poisoning; toxicity <i>adiponitrile</i>; <i>adn</i> Inhalation toxicity of adiponitrile in rats PMID 7179283; DOI 10.1016/0041-008x(82)90008-4; Toxicology and Applied Pharmacology 1982-09-15 Name matches: toxicity <i>adiponitrile</i>	
Polyploidy	4 articles	View All 
	Relationships between toxicity and structure of aliphatic nitriles*1 PMID 3803764; DOI 10.1016/0272-0590(86)90119-3; Fundamental and applied toxicology : official journal of the Society of Toxicology 1986-11-01 Name matches: homologous <i>adiponitrile</i> Substitution Reactions in Dinuclear Ru-Hbpp Complexes: an Evaluation of Through-Space Interactions PMID 22242940; DOI 10.1021/ic202225g; Inorganic Chemistry 2012-01-13 Name matches: homologous <i>adiponitrile</i> Real-time PCR detection of Fe-type nitrile hydratase genes from environmental isolates suggests horizontal gene transfer between multiple genera PMID 20502965; DOI 10.1007/s10482-010-9459-8; Antonie van Leeuwenhoek 2010-05-26	
Weight Gain	2 articles	View All 
	13-week inhalation toxicity study and fertility assessment in rats exposed to atmospheres containing adiponitrile PMID 2366257; DOI 10.1080/15287399009531423; Journal of Toxicology and Environmental Health 1990-07-01 Name matches: weight gain <i>adiponitrile</i> Toxicology and carcinogenesis studies of acrylonitrile (CAS No. 107-13-1) in B6C3F1 mice (gavage studies) PMID 11803701; National Toxicology Program technical report series 2001-10-01 Name matches: weight gain <i>adiponitrile</i>	

13.8 Chemical-Organism Co-Occurrences in Literature



Showing 3 of 62 View More



Organism	Selected evidence
rhodococcus erythropolis ccm2595	3 articles View All High Regioselectivity Production of 5-Cyanovaleramide from Adiponitrile by a Novel Nitrile Hydratase Derived from Rhodococcus erythropolis CCM2595 PMID 32743216; DOI 10.1021/acsomega.0c02188; ACS Omega 2020-07-15 Name matches: rhodococcus erythropolis ccm2595 adiponitrile Modification of nitrile hydratase from Rhodococcus erythropolis CCM2595 by semirational design to enhance its substrate affinity PMID 36456206; DOI 10.1116/6.0002061; Biointerphases 2022-11-01 Name matches: rhodococcus erythropolis ccm2595 adiponitrile Reprogramming regioselectivity of nitrile hydratase towards adiponitrile via semi-rational design of a key "switch" residue PMID 41865929; DOI 10.1016/j.ijbiomac.2026.151582; International Journal of Biological Macromolecules 2026-04-01 Name matches: rhodococcus erythropolis ccm2595 adiponitrile; adn
nita	3 articles View All Aliphatic nitrilase from a soil-isolated comamonas testosteroni sp.: gene cloning and overexpression, purification and primary structure PMID 7642130; DOI 10.1016/0378-1119(95)00242-x; Gene 1995-08-08 Name matches: nita adiponitrile Investigative mining of sequence data for novel enzymes: A case study with nitrilases PMID 19539670; DOI 10.1016/j.jbiotec.2009.06.004; Journal of Biotechnology 2009-08-10 Name matches: nita adiponitrile Conversion of aliphatic nitriles by the arylacetonitrilase from Pseudomonas fluorescens EBC191 PMID 29896645; DOI 10.1007/s11274-018-2477-9; World Journal of Microbiology and Biotechnology 2018-06-12

[brevibacterium sp.](#)

2 articles

[View All](#) **N-terminal amino acid sequence of mutant strain *Brevibacterium sp.* adipamidase**PMID 8274001; DOI 10.1007/bf00870919; Antonie van Leeuwenhoek 1993-03-01
Name matches: *brevibacterium sp. adiponitrile***Purification and Characterization of an Adipamidase from a Mutant Strain of *Brevibacterium sp.* Involved in Dinitrile Degradation**PMID 27314785; DOI 10.1271/bbb.57.294; Bioscience, Biotechnology, and Biochemistry 1993-01-01
Name matches: *brevibacterium sp. adiponitrile*[► PubChem](#)

14 Patents



14.1 Depositor-Supplied Patent Identifiers



37,096 items



SORT BY

Priority Date - Most Recent

**Method for preparing adiponitrile from cyclohexanone catalyzed by phosphorus and nitrogen co-doped porous carbon/CoP composite material**Publication Number: [CN-120757467-A](#)

Priority Date: 2025-09-05

A deep treatment system for adiponitrile waste residue oilPublication Number: [CN-120648488-A](#)

Priority Date: 2025-06-27

Advanced treatment method of adiponitrile waste residual oilPublication Number: [CN-120775612-A](#)

Priority Date: 2025-06-27

Adiponitrile hydrogenation catalyst and preparation method thereofPublication Number: [CN-120662315-A](#)

Priority Date: 2025-06-17

A green method for synthesizing hexamethylenediamine

Publication Number: [CN-120664972-A](#)

Priority Date: 2025-06-11

« First < Previous Page 1 of 7,420 Next > Last »

► [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>

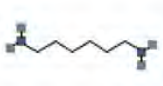
► [PATENTSCOPE \(WIPO\)](#)

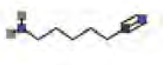
14.3 Chemical Co-Occurrences in Patents



Showing 3 of 100 [View More](#)



Chemical	Selected evidence
 Hexamethylenediamine CID 16402	986 patents from 674 patent families View All Hydrogenation of adiponitrile US-3758584-A; Grant Date: 1973-09-11 Process for preparation of polyamide from dinitrile and diamine US-6103863-A; Grant Date: 2000-08-15 Preparation of hexamethylene diamine from 2-cyanocyclopentanone and adiponitrile US-4042629-A; Grant Date: 1977-08-16

 Succinonitrile CID 8062	2,084 patents from 1,365 patent families View Top 1000 Method for manufacturing compounds including nitrile functions US-8501979-B2; Grant Date: 2013-08-06 Electrochemical cell with TMCCC electrodes in an acetonitrile solvent including a dinitrile additive US-11495831-B2; Grant Date: 2022-11-08 Method for the selective hydrogenation of a dinitrile compound US-5844114-A; Grant Date: 1998-12-01
 6-Aminohexanenitrile CID 17079	469 patents from 261 patent families View All Preparation of aliphatic alpha, omega-aminonitriles US-5512697-A; Grant Date: 1996-04-30 Separation of 6-aminocapronitrile and hexamethylenediamine from a mixture comprising hexamethylenediamine, 6-aminocapronitrile and tetrahydroazepine US-7468119-B2; Grant Date: 2008-12-23 Method for making caprolactam from impure ACN in which THA is not removed until after caprolactam is produced US-6858728-B2; Grant Date: 2005-02-22

► [PubChem](#)

14.4 Chemical-Disease Co-Occurrences in Patents



Showing 3 of 100 View More 		
Disease	Selected evidence	
Headache	8 patents from 7 patent families	View All 
	Separation of 6-aminocapronitrile and hexamethylenediamine from a mixture comprising hexamethylenediamine, 6-aminocapronitrile and tetrahydroazepine US-7468119-B2; Grant Date: 2008-12-23	
	Separation of 6-aminocapronitrile and hexamethylenediamine from a mixture comprising hexamethylenediamine, 6-aminocapronitrile and tetrahydroazepine US-7208632-B2; Grant Date: 2007-04-24	

Purification of organic nitriles US-2570794-A; Grant Date: 1951-10-09		
Immune Reconstitution Inflammatory Syndrome	6 patents from 6 patent families	View All
	Methods for cleaning recyclable substrates or containers US-8153577-B2; Grant Date: 2012-04-10	
	The use of protective biodegradable coatings for preventing the deposit of overspray EP-2462200-B1; Grant Date: 2015-11-11	
	Automatic emulsification cleaning formulation and usage JP-5695066-B2; Grant Date: 2015-04-01	
Arthrogryposis multiplex congenita neurogenic type	1 patent from 1 patent family	View All
	Electrocatalytic hydrogenations of nitriles to amines US-5266731-A; Grant Date: 1993-11-30	

► [PubChem](#)

14.5 Chemical-Gene Co-Occurrences in Patents



Showing 3 of 100 View More			
Gene	Selected evidence		
nitrile hydratase	84 patents from 43 patent families	View All	
	Polypeptides possessing a nitrilase activity and method of converting nitriles to carboxylates by means of said polypeptides US-5629190-A; Grant Date: 1997-05-13		
	Recombinant nitrilase and use thereof EP-0596812-B1; Grant Date: 1997-10-01		
	Method for producing amide compounds using a nitrile hydratase from a thermophilic bacillus US-6228633-B1; Grant Date: 2001-05-08		
amidase	48 patents from 23 patent families	View All	

Method for producing amide compounds using a nitrile hydratase from a thermophilic bacillus

US-6228633-B1; Grant Date: 2001-05-08

Polypeptides possessing a nitrilase activity and method of converting nitriles to carboxylates by means of said polypeptides

US-5629190-A; Grant Date: 1997-05-13

A process for the preparation of enantiomeric 2-alkanoic acids

EP-0549710-B1; Grant Date: 1996-02-28

litaf**30 patents from 28 patent families****View All** **Non-aqueous electrolyte and non-aqueous electrolyte secondary battery using the same**

JP-6319024-B2; Grant Date: 2018-05-09

Non-aqueous electrolyte solution and non-aqueous electrolyte secondary battery employing the same

KR-101457320-B1; Grant Date: 2014-11-04

Method for producing nonaqueous electrolyte secondary cell

KR-101848577-B1; Grant Date: 2018-04-12

 **PubChem****14.6 Chemical-Organism Co-Occurrences in Patents**Showing 3 of 100 **View More** **Organism****Selected evidence****pensacola****25 patents from 24 patent families****View All** **Reduction of diaminocyclohexane concentration in crude hexamethylenedi-amine**

US-3235600-A; Grant Date: 1966-02-15

Process for the production of hexamethylenediamine

US-3152186-A; Grant Date: 1964-10-06

Process for catalytic hydrogenation of adiponitrile

US-3272867-A; Grant Date: 1966-09-13

brevibacterium	50 patents from 27 patent families	View All
Recombinant nitrilase and use thereof EP-0596812-B1; Grant Date: 1997-10-01		
Enzymatic process EP-0178106-B1; Grant Date: 1993-03-31		
Process for the preparation of amides by biological hydrolysis US-4001081-A; Grant Date: 1977-01-04		
corynebacterium	65 patents from 36 patent families	View All
Recombinant nitrilase and use thereof EP-0596812-B1; Grant Date: 1997-10-01		
Polypeptides possessing a nitrilase activity and method of converting nitriles to carboxylates by means of said polypeptides US-5629190-A; Grant Date: 1997-05-13		
A process for the preparation of enantiomeric 2-alkanoic acids EP-0549710-B1; Grant Date: 1996-02-28		

► [PubChem](#)

15 Interactions and Pathways



15.1 Chemical-Target Interactions



39 items					
Search			SORT BY Data Source - A to Z		
Protein	Gene	Taxonomy	Action	Evidence	Data Source
Glutathione reductase, mitochondrial	GSR	Homo sapiens (human)	Cyanide inhibits glutathione reductase. (A76)	PMID:2734799	Toxin and Toxin Target Database (T3DB)

Cytochrome c oxidase subunit 1	COX1	Homo sapiens (human)	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. (L97)	Toxin and Toxin Target Database (T3DB)
Cytochrome c oxidase subunit 4 isoform 1, mitochondrial	COX4I1	Homo sapiens (human)	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. (L97)	Toxin and Toxin Target Database (T3DB)
Cytochrome c oxidase subunit 7A1, mitochondrial	COX7A1	Homo sapiens (human)	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,	Toxin and Toxin Target Database (T3DB)

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. (L97)

Cytochrome c
oxidase
subunit 7B2,
mitochondrial

COX7B2

Homo
sapiens
(human)

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. (L97)

Toxin and
Toxin
Target
Database
(T3DB)

« First < Previous Page 1 of 8 Next > Last »

► Toxin and Toxin Target Database (T3DB)

16 Biological Test Results



16.1 BioAssay Results



1,184 items



SORT BY Activity Value - Increasing



Cytochrome P450 Family 2 Subfamily C Member 9 (CYP2C9) small molecule antagonists:
luciferase reporter qHTS assay

Activity Outcome: Unspecified Activity Type: Potency Activity Value: 0.002500 µM

BioAssay AID: 1671198

Target Name: [CYP2C9 - cytochrome P450 family 2 subfamily C member 9 \(human\)](#)

Substance SID: [144210346](#) Compound CID: [8128](#)

Cytochrome P450 Family 2 Subfamily C Member 9 (CYP2C9) small molecule antagonists: luciferase reporter qHTS assay

Activity Outcome: [Unspecified](#) Activity Type: Potency Activity Value: 0.002500 µM

BioAssay AID: [1671198](#)

Target Name: [CYP2C9 - cytochrome P450 family 2 subfamily C member 9 \(human\)](#)

Substance SID: [144210346](#) Compound CID: [8128](#)

A CellTox Green Cytotoxicity Assay to monitor cytotoxicity in HepG2 cells - 24 hour

Activity Outcome: [Unspecified](#) Activity Type: Potency Activity Value: 0.173700 µM

BioAssay AID: [1224878](#)

Substance SID: [144210346](#) Compound CID: [8128](#)

A CellTox Green Cytotoxicity Assay to monitor cytotoxicity in HepG2 cells - 16 hour

Activity Outcome: [Unspecified](#) Activity Type: Potency Activity Value: 0.194900 µM

BioAssay AID: [1224876](#)

Substance SID: [144210346](#) Compound CID: [8128](#)

A CellTox Green Cytotoxicity Assay to monitor cytotoxicity in HepG2 cells - 32 hour

Activity Outcome: [Unspecified](#) Activity Type: Potency Activity Value: 0.194900 µM

BioAssay AID: [1224883](#)

Substance SID: [144210346](#) Compound CID: [8128](#)

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► [PubChem](#)

17 Classification



17.1 MeSH Tree



1 item

[View in Classification Browser](#)

MeSH Tree > Chemicals and Drugs Category > Organic Chemicals > Nitriles

[adiponitrile](#)

MeSH Concept: [M0111245](#)
MeSH Descriptor: [C036546](#)

► **Medical Subject Headings (MeSH)**

17.2 ChemIDplus



45 itemsView in Classification Browser

[ChemIDplus Chemical Information Classification > Other Resources \(Internet Locators\)](#)
CAMEO
Computer-Aided Management of Emergency Operation - CAMEO Chemicals is a library of datasheets containing response-related information and recommendations for hazardous materials that are commonly transported, used, or stored in the United States

[ChemIDplus Chemical Information Classification > NLM Resources \(File Locators\)](#)
CCRIS
Chemical Carcinogenesis Research Information System - Carcinogenicity, mutagenicity, tumor promotion and tumor inhibition data from the National Cancer Institute (NCI). CCRIS provides historical information from the years 1985 - 2011. It is no longer updated.

[ChemIDplus Chemical Information Classification > Regulatory Agencies \(Superlist Locators\)](#)
CGB
Coast Guard Bulk Hazardous Materials - Coast Guard Bulk Hazardous Materials. Hazardous Materials Standards Division, Coast Guard, U.S. Department of Homeland Security

[ChemIDplus Chemical Information Classification > Regulatory Agencies \(Superlist Locators\)](#)
CGN
Coast Guard Noxious Liquid Substances - Coast Guard Noxious Liquid Substances. Hazardous Materials Standards Division, Coast Guard, U.S. Department of Homeland Security

[ChemIDplus Chemical Information Classification > Other Resources \(Internet Locators\)](#)
CTD
Comparative Toxicogenomics Database - CTD selects and organizes gene, sequence, chemical, reference, and

« First < Previous Page 1 of 9 Next > Last »

[► ChemIDplus](#)

17.3 CAMEO Chemicals



1 item	View in Classification Browser
CAMEO Chemical Reactivity Classification	
Nitriles	
Reactive group: Nitriles	

[► CAMEO Chemicals](#)

17.4 UN GHS Classification



52 items	View in Classification Browser
GHS Classification > Hazard Statement Codes > H300: Health Hazards	
H301: Toxic if swallowed [<u>Danger</u> : Acute toxicity, oral]	
GHS Classification > Hazard Statement Codes > H300: Health Hazards	
H311: Toxic in contact with skin [<u>Danger</u> : Acute toxicity, dermal]	
GHS Classification > Hazard Statement Codes > H300: Health Hazards	
H313: May be harmful in contact with skin [<u>Warning</u> : Acute toxicity, dermal]	
GHS Classification > Hazard Statement Codes > H300: Health Hazards	
H315: Causes skin irritation [<u>Warning</u> : Skin corrosion/irritation]	
GHS Classification > Hazard Statement Codes > H300: Health Hazards	
H319: Causes serious eye irritation [<u>Warning</u> : Serious eye damage/eye irritation]	
« First < Previous Page 1 of 11 Next > Last »	

[► GHS Classification \(UNECE\)](#)

17.5 EPA Chemical Data Reporting Classification



4 items	View in Classification Browser
EPA Chemical Data Reporting Classification > Industry Uses	
Intermediate	
Industry use category: Intermediate	
EPA Chemical Data Reporting Classification > Industry Uses	
Other	
Industry use category: Other	
EPA Chemical Data Reporting Classification > Industry Processing Sectors	
Services	
Industry Processing Sector: Services	
EPA Chemical Data Reporting Classification > Industry Processing Sectors	
All Other Basic Organic Chemical Manufacturing	
Industry Processing Sector: All Other Basic Organic Chemical Manufacturing	

► [EPA Chemical Data Reporting \(CDR\)](#)

17.6 NORMAN Suspect List Exchange Classification



27 items	View in Classification Browser
NORMAN Suspect List Exchange Classification	
S00 SUSDAT Merged NORMAN Suspect List: SusDat	
A merged list of > 100,000 structures from the NORMAN Network Suspect List Exchange, available from https://www.norman-network.com/nds/susdat/ . Compiled by Reza Aalizadeh, University of Athens, including RTI and toxicity values, support by Nikiforos Alygizakis, EI. Hazard and Exposure values provided by Stellan Fischer, KEMI. Dataset DOI:10.5281/zenodo.2664077	
NORMAN Suspect List Exchange Classification	
S01 MASSBANK NORMAN Compounds in MassBank EU	

A list of NORMAN contributions to MassBank.EU (www.massbank.eu), typically processed with RMassBank (Stravs et al. 2013, DOI:10.1002/jms.3131). Dataset DOI:10.5281/zenodo.2621390

NORMAN Suspect List Exchange Classification

S02 | STOFFIDENT | HSWT/LfU STOFF-IDENT Database of Water-Relevant Substances

The STOFF-IDENT database enables the search for exact masses from target or unknown lists and the automatic use of a Retention Time Index. See <https://water.for-ident.org/#!home> (single search for free; batch search after free registration). Dataset DOI:10.5281/zenodo.2621451

NORMAN Suspect List Exchange Classification

S17 | KEMIMARKET | Swedish Chemical Agency (KEMI) Market List

List of chemicals on the market from the Swedish Chemicals Agency (KEMI). Provided by Stellan Fischer, KEMI including Hazard and Exposure scores. Curated by Reza Aalizadeh, University of Athens. Dataset DOI:10.5281/zenodo.2628786

NORMAN Suspect List Exchange Classification

S27 | KWRSJERPS2 | Extended Suspect List from Sjerps et al (KWRSJERPS)

« First < Previous Page 1 of 6 Next > Last »

► NORMAN Suspect List Exchange

17.7 EPA DSSTox Classification



96 items

View in Classification Browser

CompTox Chemicals Dashboard Chemical Lists > LIST

⌵ Show alternative paths

[40CFR355] 40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities

Short_Description: Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378)

CompTox Chemicals Dashboard Chemical Lists > LIST

⌵ Show alternative paths

[BLOODEXPOSOME] LIST: BLOODEXPOSOME Chemicals identified as part of the blood exposome

Short_Description: Chemicals identified as part of the blood exposome

[CompTox Chemicals Dashboard Chemical Lists](#) > [LIST](#)[Show alternative paths](#)

[\[BMDHHA\] ARTICLE; Bench-Mark Dose Human Health Assessment List \(Wignall et al., 2014\)](#)

Short_Description: Chemicals associated with the article "Standardizing Benchmark Dose Calculations to Improve Science-Based Decisions in Human Health Assessments" by Wignall et al., 2014

[CompTox Chemicals Dashboard Chemical Lists](#) > [LIST](#)[Show alternative paths](#)

[\[CANADADSL\] Canadian Domestic Substances List 2019](#)

Short_Description: The domestic substances list (DSL) is the sole standard against which a substance is judged to be "new" to Canada.

[CompTox Chemicals Dashboard Chemical Lists](#) > [LIST](#)[Show alternative paths](#)

« First < Previous Page 1 of 20 Next > Last »

[▶ EPA DSSTox](#)

17.8 EPA TSCA and CDR Classification



1 item

[View in Classification Browser](#)[EPA TSCA Classification](#) > [Commercial Activity Status](#)

ACTIVE

Commercial Activity Status: ACTIVE

[▶ EPA Chemicals under the TSCA](#)

17.9 EPA Substance Registry Services Tree



37 items

[View in Classification Browser](#)[EPA SRS List Classification](#) > [Ad Hoc](#)

Regional Screening Levels

RSL :: The RSL website is now the source of screening levels for all the EPA regions. The RSL tables provide comparison values for residential and commercial/industrial exposures to soil, air, and tapwater (drinking water). The unified use of the RSLs, to screen chemicals at Superfund sites, promotes national consistency. Here you will find tables of risk-based screening levels, calculated using the latest toxicity values, default exposure assumptions and physical and chemical properties, and a calculator where default parameters can be changed to reflect site-specific risks.

EPA SRS List Classification > Ad Hoc

Synonyms Provided by Submitters to the TSCA Inventory

TSCA INV SYN :: Synonyms Provided by Submitters to the TSCA Inventory

EPA SRS List Classification > EPA Application/System

2012 Chemical Data Reporting

2012 CDR :: This list contains chemicals that were reported to EPA's 2012 Chemical Data Reporting (CDR). Companies that manufacture (including import) certain chemicals at certain volumes in the U.S. must report to EPA every four years through its CDR. The vast majority of chemicals on this 2012 CDR list needed to be reported, but some of these chemicals were not required to be reported. EPA uses the CDR data to support many health, safety, and environmental protection activities.

EPA SRS List Classification > EPA Application/System

CAMEO Chemicals

CAMEO Chemicals is an emergency response and planning tool. This program includes an extensive chemical database with critical response information for thousands of chemicals, as well as a reactivity prediction tool that allows you to see what hazards might occur if chemicals in your collection were mixed together. CAMEO Chemicals is available as a website, mobile website, and a desktop application. CAMEO Chemicals is part of a software suite of programs called CAMEO (Computer-Aided Management of Emergency Operations). The CAMEO suite also includes a hazard modeling tool (ALOHA), a mapping program (MARPLOT), and two database applications (CAMEOfm and Tier2 Submit) designed to assist with the data management requirements under the Emergency Planning and Community Right-to-Know Act (EPCRA, also known as SARA Title III). The CAMEO suite programs can be used (individually or together) to help first responders and emergency planners access and manage crucial chemical property and emergency response information for hazardous chemical releases. The CAMEO programs are developed jointly by EPA's Office of Emergency Management and NOAA's Office of Response and Restoration.

EPA SRS List Classification > EPA Application/System

Chemicals On Reporting Rules

[First](#)
[Previous](#)
Page **1** of 8
 [Next](#)
[Last](#)

► [EPA Substance Registry Services](#)

17.10 MolGenie Organic Chemistry Ontology



9 items

[View in Classification Browser](#)

MolGenie Organic Chemistry Ontology > PubChemLite chemical entities > substructural concepts >

functional groups > nitrogen containing functional groups

nitriles

MolGenie Organic Chemistry Ontology > PubChemLite chemical entities > calculated properties > compound with effects on reproductive system

known reproductive effects

MolGenie Organic Chemistry Ontology > ChEMBL chemical entities > substructural concepts > functional groups > nitrogen containing functional groups

nitriles

MolGenie Organic Chemistry Ontology > ChEMBL chemical entities > calculated properties > compound with effects on reproductive system

known reproductive effects

MolGenie Organic Chemistry Ontology > PubChemLite chemical entities > compounds > organic compounds

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▶ MolGenie

17.11 Chemicals in PubChem from Regulatory Sources



10 items

View in Classification Browser

Chemicals in PubChem from Regulatory Sources > Australian Industrial Chemicals Introduction Scheme (AICIS)

Industrial Chemicals Inventory

The Australian Inventory of Industrial Chemicals (Inventory) contains information about the chemical identity and regulatory obligations relating to the importation and manufacture of industrial chemicals in Australia.

Chemicals in PubChem from Regulatory Sources > US EPA > EPA Chemical Data Reporting

Consumer Uses

Chemicals in PubChem from Regulatory Sources > US EPA > EPA Chemical Data Reporting

Industry Processing

Chemicals in PubChem from Regulatory Sources > US EPA > EPA Chemical Data Reporting

Industry Uses

Chemicals in PubChem from Regulatory Sources > US EPA

EPA Integrated Risk Information System (IRIS)

Chemical listed in the EPA Integrated Risk Information System (IRIS)

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18 Information Sources



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Hexanedinitrile

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https://chemicalsafety.ilo.org/dyn/icsc/showcard.display?p_card_id=0211

4. PAC Chemical Database, U.S. Department of Energy