

11/13/22, 5:40 PM

Sucrose | C₁₂H₂₂O₁₁ - PubChem



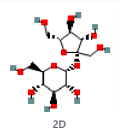
COMPOUND SUMMARY

Sucrose

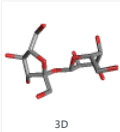
PubChem CID

5988

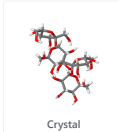
Structure



2D



3D



Crystal

[Find Similar Structures](#)

Chemical Safety

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

Molecular Formula

C₁₂H₂₂O₁₁

Synonyms

sucrose

57-50-1

saccharose

Table sugar

Cane sugar

[More...](#)

Molecular Weight

342.30

Dates

Modify

2022-11-12

Create

2004-09-16

Sucrose appears as white odorless crystalline or powdery solid. Denser than [water](#).

[▶ CAMEO Chemicals](#)

Sucrose is a glycosyl glycoside formed by [glucose](#) and [fructose](#) units joined by an acetal oxygen bridge from hemiacetal of [glucose](#) to the hemiketal of the [fructose](#). It has a role as an osmolyte, a sweetening agent, a human metabolite, an algal metabolite, a *Saccharomyces cerevisiae* metabolite, an *Escherichia coli* metabolite and a mouse metabolite.

[▶ ChEBI](#)

Sucrose is a metabolite found in the aging [mouse](#) brain.

[▶ West Coast Metabolomics Center-UC Davis](#)

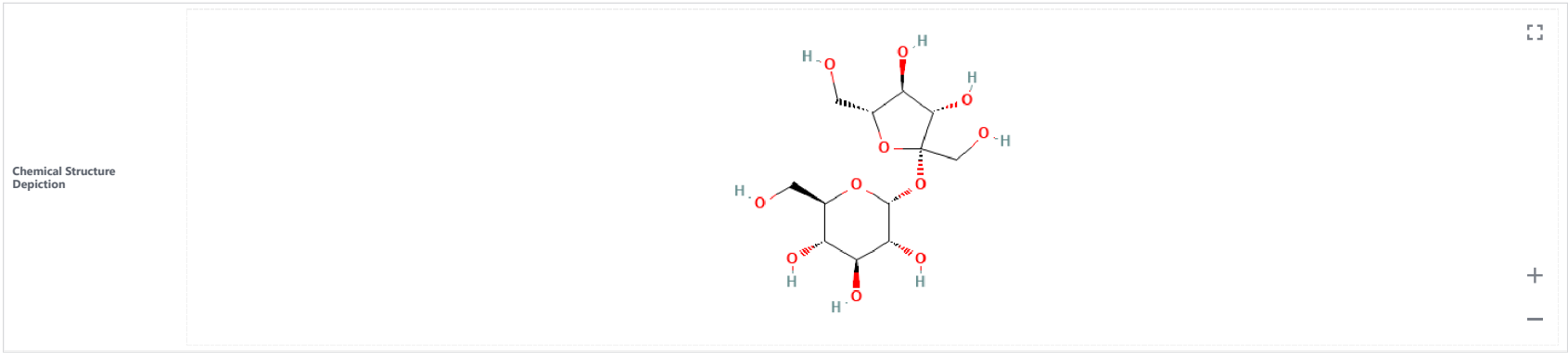
11/13/22, 5:40 PM

Sucrose | C₁₂H₂₂O₁₁ - PubChem

1 Structures



1.1 2D Structure



► PubChem

1.2 3D Conformer



► PubChem

1.3 Crystal Structures



Showing 1 of 29 View More

CCDC Number	156796
Crystal Structure Data	DOI:10.5517/cc584yh
Crystal Structure Depiction	

► The Cambridge Structural Database

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Sucrose | C12H22O11 - PubChem

2 Biologic Description



SVG Image

IUPAC Condensed	Glc(a1-2b)Fruf
LINUCS	[] [a-D-Glcp] {}
IUPAC	beta-D-arabino-hex-2-ulofuranosyl alpha-D-gluco-hexopyranoside
WURCS	WURCS=2.0/2,2,1/[a2122h-1a_1-5][ha122h-2b_2-5]/1-2/a1-b2

▶ [PubChem](#)

GlyCosmos Monoisotopic Mass	342.12
GlyCosmos Subsumption	Linkage defined saccharide

▶ [GlyCosmos Glycoscience Portal](#)

3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

(2R,3R,5S,6S,6R)-2-((2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl)oxy-6-(hydroxymethyl)oxane-3,4,5-triol
Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

3.1.2 InCHI

inChI=1S/C12H22O11/C13-1-4-6(16)8(18)9(11)12(14)23-12(3-15)10(20)7(17)5(2-14)22-12(4-11)13-20H1-3H2/4-5-6-7-8+9-10+11-12+/m1/s1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

3.1.3 InChIkey

CZMRCDWAGMRECN-UGDNZRGBSA-N

Computed by InChI 1.0.6 (PubChem release 2019.07.25)

PubChem

3.1.4 Canonical SMILES

PubChem

3.1.5 Isomeric SMILES

PubChem
Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

3.2 Molecular Formula

► CAMEO Chemicals; ILO International Chemical Safety Cards (ICSC); PubChem

3.3 Other Identifiers

3.3.1 CAS

57-50-1

▶ CAMERO Chemicals; CA5 Common Chemistry; ChemIDplus; DrugBank; EPA Chemicals under the TSCA; EPA D55Tox; European Chemicals Agency (ECHA); FDA Global Substance Registration System (GSRS); Hazardous Substances Data Bank (HSDB); Human Metabolome Database (HMDB); ILO International Labour Organization (ILO)

▶ European Chemicals Agency (ECHA)



3.3.2 Related CAS

25702-74-3

Compound: Polysucrose

CAS Common Chemistry



3.3.3 Deprecated CAS

ChemIDplus

100405-08-1, 104242-10-6, 131932-12-2, 146187-04-4, 151756-02-4, 220376-22-7, [29253-78-9](#), 29764-06-5, 30027-72-6, 47167-52-2, 47185-09-1, 47257-91-0, 50857-68-6, 51909-69-4, 64533-66-0, 65545-99-5, 75398-84-4, 76056-38-7, 78654-77-0, 80165-03-3, 8027-47-2, 8030-20-4, 85456-51-5, 86101-30-6, 87430-66-8, 92004-84-7, 935681-90-2, 786702-63-4, 12040-73-2, 1159795-78-4, 1206156-82-2, 880257-62-5, [1192061-43-0](#), 1481578-88-4, 1566560-95-9, 2169316-40-7

EPA DSSTox

100405-08-1, 104242-10-6, 1159795-78-4, 12040-73-2, 1206156-82-2, 131932-12-2, 146054-35-5, 146187-04-4, 151756-02-4, 220376-22-7, [29253-78-9](#), 29764-06-5, 30027-72-6, 47167-52-2, 47185-09-1, 47257-91-0, 50857-68-6, 51909-69-4, 635681-90-2, 64533-66-0, 65545-99-5, 75398-84-4, 76056-38-7, 78654-77-0, 786702-63-4, 80165-03-3, 8027-47-2, 8030-20-4, 85456-51-5, 86101-30-6, 87430-66-8, 880257-62-5, 92004-84-7



3.3.4 European Community (EC) Number

200-334-9

European Chemicals Agency (ECHA)

618-806-1

European Chemicals Agency (ECHA)



3.3.5 ICSC Number

1507

ILO International Chemical Safety Cards (ICSC)



3.3.6 RTECS Number

WN6500000

The National Institute for Occupational Safety and Health (NIOSH)



3.3.7 UNII

C151H8M554

FDA Global Substance Registration System (GSRS)



3.3.8 DSSTox Substance ID

DTXSID2021288

EPA DSSTox



3.3.9 Wikidata

Q4027534

Wikidata

<https://pubchem.ncbi.nlm.nih.gov/compound/5988>

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3.3.10 GlyTouCan Accession



- G05551OP
 - GlyCosmos Glycoscience Portal; GlyTouCan Project
- G78152OD
 - GlyTouCan Project
- G44791DH
 - GlyTouCan Project

3.3.11 NCI Thesaurus Code



- C68477
 - NCI Thesaurus (NCIt)

3.3.12 RXCUI



- 10159
 - NLM RxNorm Terminology

3.4 Synonyms



3.4.1 MeSH Entry Terms



Saccharose
Sucrose

Medical Subject Headings (MeSH)

3.4.2 Depositor-Supplied Synonyms



sucrose	Granulated sugar	Sucraloxum [INN-Latin]	(+)-Sucrose	DSSTox_CID_1288
57-50-1	Rock candy	beta-D-Fructofuranosyl-alpha-D-glucopyranoside	alpha-D-Glucopyranoside, beta-D-fructofuranosyl-	NSC 406942
saccharose	Amerfand	D-(-)-Saccharose	NCI-C56597	DSSTox_RID_76060
Table sugar	Amerfond	CCRIS 2120	GNE-410	DSSTox_GSID_21288
Cane sugar	Confectioner's sugar	HSDB 500	S-67F	Polysucrose
White sugar	D(+)-Sucrose	Sacharose	1-alpha-D-glucopyranosyl-2-beta-D-fructofuranoside	(2R,3R,4S,5S,6R)-2-[[[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy]-6-(hydroxymethyl)oxane-3,
D-Sucrose	Sucrose, dust	alpha-D-Glucopyranosyl beta-D-fructofuranoside	alpha-D-Glucopyranoside, beta-D-fructofuranosyl	Sucrose [USAN:JAN]
Saccharum	Sucrose, pure	CHEBI:17992	C151H8M554	D-Saccharose
sugar	D(+)-Saccharose	AI3-09085	NSC-406942	MFCDD00006626
Rohrzucker	sacarosa	(alpha-D-Glucosido)-beta-D-fructofuranoside	beta-D-Fruf-(2<->1)-alpha-D-Glcp	CAS-57-50-1
Microse	D-(-)-Sucrose	Fructofuranoside, alpha-D-glucopyranosyl, beta-D	NCGC00164248-01	(2R,3R,4S,5S,6R)-2-[[[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy]-6-(hydroxymethyl)oxane-
Beet sugar	beta-D-Fructofuranosyl alpha-D-glucopyranoside	Glucopyranoside, beta-D-fructofuranosyl, alpha-D	Sucraloxum	Sucrose [JAN:NF]

PubChem

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Sucrose | C12H22O11 - PubChem

4 Chemical and Physical Properties



4.1 Computed Properties



Property Name	Property Value	Reference
Molecular Weight	342.30	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3	-3.7	Computed by XLogP3 3.0 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	8	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	11	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Rotatable Bond Count	5	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	342.11621151	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	342.11621151	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	190 Å²	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	23	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	395	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	9	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.05.07)

► PubChem

4.2 Experimental Properties



4.2.1 Physical Description



Sucrose appears as white odorless crystalline or powdery solid. Denser than [water](#).

► CAMEO Chemicals

Liquid; OtherSolid; OtherSolid, Liquid; PelletsLargeCrystals; WetSolid

► EPA Chemicals under the TSCA

Hard, white, odorless crystals, lumps, or powder. [Note: May have a characteristic, caramel odor when heated.]; [NIOSH]

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

Solid

► Human Metabolome Database (HMDB)

WHITE SOLID IN VARIOUS FORMS.

► ILO International Chemical Safety Cards (ICSC)

Hard, white, odorless crystals, lumps, or powder.

► Occupational Safety and Health Administration (OSHA)

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Hard, white, odorless crystals, lumps, or powder. [Note: May have a characteristic, caramel odor when heated.]

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

4.2.2 Color/Form



Monoclinic sphenoidal crystals, crystalline masses, blocks, or powder

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1517

▶ Hazardous Substances Data Bank (HSDB)

Hard, white ... crystals, lumps, or powder ...

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 288

▶ Hazardous Substances Data Bank (HSDB)

4.2.3 Odor



Characteristic caramel

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1518

▶ Hazardous Substances Data Bank (HSDB)

... Odorless ... [Note: May have a characteristic caramel odor when heated].

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 288

▶ Hazardous Substances Data Bank (HSDB)

4.2.4 Taste



Sweet

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1517

▶ Hazardous Substances Data Bank (HSDB)

4.2.5 Boiling Point



Decomposes (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

decomposes

▶ Occupational Safety and Health Administration (OSHA)

Decomposes

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

4.2.6 Melting Point



320 to 367 °F (decomposes) (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

185.5 °C

PhysProp

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▶ [DrugBank](#)

185.5 °C

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., 1998-1999, p. 3-172

▶ [Hazardous Substances Data Bank \(HSDB\)](#); [Human Metabolome Database \(HMDB\)](#)

320-367 °F (decomposes)

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

320-367 °F (Decomposes)

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

4.2.7 Solubility



greater than or equal to 100 mg/mL at 66 °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](#)

2100000 mg/L (at 25 °C)

YALKOWSKY,SH & DANNENFELSER,RM (1992)

▶ [DrugBank](#)

1 g dissolves in 0.5 ml [water](#), 170 ml alcohol, about 100 ml [methanol](#). Moderately sol in [glycerol](#), [pyridine](#).

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996, p. 1518

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

Very soluble in [water](#), [methanol](#); slightly soluble in [ethanol](#); insoluble in [ethyl ether](#).

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., 1998-1999, p. 3-172

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

[water](#) solubility = 2.12X10+6 mg/l @ 25 °C

Yalkowsky SH, Dannenfelser RM; The AQUASOL dATABASE of Aqueous Solubility. Fifth Ed, Tucson, AZ: Univ Az, College of Pharmacy (1992)

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

2100.0 mg/mL

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

Solubility in [water](#), g/100ml at 25 °C: 200

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

200%

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

4.2.8 Density



1.59 at 68 °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](#)

1.5805 g/cu cm @ 17 °C

<https://pubchem.ncbi.nlm.nih.gov/compound/5988>

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Sucrose | C12H22O11 - PubChem

Lide, D.R. (ed.). *CRC Handbook of Chemistry and Physics*. 79th ed. Boca Raton, FL: CRC Press Inc., 1998-1999, p. 3-172

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

1.6 g/cm³

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

1.59

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

4.2.9 Vapor Pressure



0 mmHg (approx) (NIOSH, 2022)

▶ [CAMEO Chemicals](#)

0 mmHg (approx)

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

4.2.10 LogP



-3.7

HANSCH, C ET AL. (1995)

▶ [DrugBank](#)

log Kow = -3.70

Hansch, C., Leo, A., D. Hoekman. *Exploring QSAR - Hydrophobic, Electronic, and Steric Constants*. Washington, DC: American Chemical Society, 1995, p. 107

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

-3.70

HANSCH, C ET AL. (1995)

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

-3.67

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

4.2.11 Stability/Shelf Life



STABLE IN AIR

The Merck Index. 9th ed. Rahway, New Jersey: Merck & Co., Inc., 1976., p. 1149

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

4.2.12 Decomposition



When heated to decomposition it emits acrid smoke and fumes.

Sax, N.I. *Dangerous Properties of Industrial Materials*. 6th ed. New York, NY: Van Nostrand Reinhold, 1984., p. 2478

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

186 °C

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

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4.2.13 Heat of Combustion



-1.35X10+6 cal/mol
Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984., p. V21 867
▶ [Hazardous Substances Data Bank \(HSDB\)](#)

4.2.14 pH



Soln are neutral to litmus
Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 1057
▶ [Hazardous Substances Data Bank \(HSDB\)](#)

4.2.15 Surface Tension



71-75 mN/m @ 1-0.6 mol/l
Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VB1 (90) 6-54
▶ [Hazardous Substances Data Bank \(HSDB\)](#)

4.2.16 Refractive Index



INDEX OF REFRACTION: 1.5376; SADTLER REFERENCE NUMBER: 8659 (IR, PRISM), 563 (IR, GRATING); SPECIFIC OPTICAL ROTATION: +66.37 @ 20 °C/D ([WATER](#))
Weast, R.C. (ed.). Handbook of Chemistry and Physics. 60th ed. Boca Raton, Florida: CRC Press Inc., 1979., p. C-503
▶ [Hazardous Substances Data Bank \(HSDB\)](#)

4.2.17 Caco2 Permeability



-5.77
ADME Research, USCD
▶ [DrugBank](#)

4.2.18 Dissociation Constants



pKa
12.6
MERCK INDEX (1996)
▶ [DrugBank](#)

pKa= 12.62
Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1518
▶ [Hazardous Substances Data Bank \(HSDB\)](#)

4.2.19 Collision Cross Section



174 Å² [M+Na]⁺ [CCS Type: DT, Method: single field calibrated with Agilent tune mix (Agilent)]
<https://pubs.acs.org/doi/abs/10.1021/acs.analchem.6b03091>
▶ [CCSbase](#)

173.93 Å² [M+Na]⁺ [CCS Type: DT, Method: stepped-field]
<https://pubs.rsc.org/en/content/articlelanding/2017/sc/c7sc03464d>
▶ [CCSbase](#)

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168.47 Å² [M-H]⁻ [CCS Type: DT, Method: stepped-field]
<https://pubs.rsc.org/en/content/articlelanding/2017/sc/c7sc03464d>
▶ CCSbase

170 Å² [M+Na]⁺ [CCS Type: TW, Method: calibrated with [polyalanine](#)]
<https://pubs.acs.org/doi/abs/10.1021/ac500405x>
▶ CCSbase

175.4 Å² [M+K]⁺ [CCS Type: DT, Method: single field calibrated with ESI Low Concentration Tuning Mix (Agilent)]
<https://pubs.acs.org/doi/abs/10.1021/acs.analchem.8b04322>
▶ CCSbase

173.9 Å² [M+Na]⁺ [CCS Type: DT, Method: single field calibrated with ESI Low Concentration Tuning Mix (Agilent)]
<https://pubs.acs.org/doi/abs/10.1021/acs.analchem.8b04322>
▶ CCSbase

168.2 Å² [M-H]⁻ [CCS Type: DT, Method: single field calibrated with ESI Low Concentration Tuning Mix (Agilent)]
<https://pubs.acs.org/doi/abs/10.1021/acs.analchem.8b04322>
▶ CCSbase

168.2 Å² [M-H]⁻
173.9 Å² [M+Na]⁺
175.5 Å² [M+K]⁺
550 | CCSCOMPEND | The Unified Collision Cross Section (CCS) Compendium | DOI:10.5281/zenodo.2658162
▶ NORMAN Suspect List Exchange

4.2.20 Other Experimental Properties



Decomp @ 160-186 °C; does not reduce Fehling's soln, form osazone, or show mutarotation; hydrolyzed to [glucose](#) and [fructose](#) by dil acids and by invertase, a yeast enzyme; upon hydrolysis optical rotation falls and is negative when hydrolysis is complete.
Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1518
▶ Hazardous Substances Data Bank (HSDB)

Surface tension of aqueous solution (0.1-0.6 mol/l) = 71-75 mN/m
Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VB1 6-54
▶ Hazardous Substances Data Bank (HSDB)

Enthalpy of formation = 86 cal/mol-deg K
Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. V21 867
▶ Hazardous Substances Data Bank (HSDB)

4.2.21 Chemical Classes



Biological Agents -> Disaccharides
▶ Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

4.3 SpringerMaterials Properties



Chemical diffusion	Sound absorption
Crystal structure	Sound propagation
Density	Sound velocity

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Diamagnetic susceptibility	Space group
Diffusion	Unit cell
Diffusive flux	Unit cell parameter
Fluorescence	
Formula unit	
Formula weight	
Kinetic properties	
Magnetic anisotropy	
Magnetic susceptibility	

► [SpringerMaterials](#)

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Sucrose | C12H22O11 - PubChem

5 Spectral Information



5.1 1D NMR Spectra



1D NMR Spectra	NMR: 6242 (Sadtler Research Laboratories Spectral Collection)
----------------	---

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

5.1.1 1H NMR Spectra



Showing 2 of 5 [View More](#)

Spectra ID	1293
Instrument Type	Varian
Frequency	500 MHz
Solvent	Water
pH	7.00
Shifts [ppm]:Intensity	3.45:14.34, 3.46:32.94, 3.48:19.73, 3.54:19.67, 3.54:19.93, 3.56:23.56, 3.56:24.20, 3.67:100.00, 3.73:22.02, 3.75:29.84, 3.77:15.98, 3.80:23.93, 3.81:84.56, 3.81:93.51, 3.83:13.15, 3.84:12.88, 3.85:5.07, 3.86:10.19, 3.87:8.15, 3.87:9.80, 3.88:13.29, 3.88:13.36, 3.88:8.83, 3.89:8.78, 3.90:7.79, 4.02:14.45, 4.04:27.23, 4.06:15.18, 4.20:28.93, 4.22:22.97, 5.39:18.49, 5.40:19.11
Thumbnail	

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

Spectra ID	3910
Instrument Type	JEOL
Frequency	400 MHz
Solvent	D2O
Shifts [ppm]:Intensity	3.45:136.00, 3.47:279.00, 3.50:200.00, 3.54:187.00, 3.56:183.00, 3.57:228.00, 3.58:235.00, 3.68:1000.00, 3.74:231.00, 3.76:267.00, 3.79:181.00, 3.80:55.00, 3.81:550.00, 3.82:854.00, 3.83:862.00, 3.84:98.00, 3.85:140.00, 3.85:99.00, 3.86:149.00, 3.87:138.00, 3.88:135.00, 3.89:140.00, 3.89:97.00, 3.90:166.00, 3.90:84.00, 3.91:96.00, 3.92:80.00, 4.03:198.00, 4.05:344.00, 4.08:207.00, 4.21:506.00, 4.23:391.00, 5.41:314.00, 5.42:308.00
Thumbnail	

11/13/22, 5:40 PM

Sucrose | C12H22O11 - PubChem



▶ Human Metabolome Database (HMDB)

5.1.2 13C NMR Spectra



Showing 2 of 5 View More

Spectra ID	1220
Instrument Type	Bruker
Frequency	125 MHz
Solvent	Water
pH	7.00
Shifts [ppm]:Intensity	0.00:1.45, 106.36:14.24, 62.89:15.61, 64.14:14.09, 65.08:18.49, 71.98:20.85, 73.80:22.62, 75.10:22.60, 75.33:21.72, 76.78:18.90, 79.24:16.27, 84.05:22.63, 94.85:21.82
Thumbnail	

▶ Human Metabolome Database (HMDB)

Spectra ID	166519
Frequency	400 MHz
Solvent	H2O
Shifts [ppm]	106.36, 62.89, 64.14, 65.08, 71.98, 73.80, 75.10, 75.33, 76.78, 79.24, 84.05, 94.85
Thumbnail	

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Sucrose | C12H22O11 - PubChem

Human Metabolome Database (HMDB)

5.2 2D NMR Spectra



5.2.1 1H-1H NMR Spectra



2D NMR Spectra Type	1H-1H TOCSY
Spectra ID	1009
Shifts [ppm] (F2:F1)	3.30:3.66, 3.39:3.66, 3.42:3.66, 3.43:3.49, 3.44:5.40, 3.46:3.43, 3.46:3.46, 3.46:3.54, 3.46:3.66, 3.46:3.73, 3.46:3.75, 3.46:3.81, 3.46:3.85, 3.47:3.78, 3.48:5.40, 3.50:3.49, 3.52:3.66, 3.53:5.40, 3.54:3.66, 3.55:3.46, 3.55:3.47, 3.55:3.54, 3.55:3.56, 3.55:3.73, 3.55:3.75, 3.55:3.78, 3.55:3.81, 3.55:3.85, 3.56:5.40, 3.58:3.66, 3.61:3.66, 3.67:3.67, 3.71:3.67, 3.71:3.72, 3.72:3.80, 3.74:3.66, 3.74:3.78, 3.75:3.43, 3.75:3.46, 3.75:3.49, 3.75:3.54, 3.75:3.55, 3.75:3.75, 3.75:3.84, 3.75:5.40, 3.80:3.72, 3.81:3.43, 3.81:3.46, 3.81:3.48, 3.81:3.53, 3.81:3.56, 3.81:3.81, 3.81:3.85, 3.81:3.88, 3.81:3.90, 3.81:4.02, 3.81:4.20, 3.81:4.22, 3.82:4.04, 3.82:4.07, 3.83:3.73, 3.83:3.75, 3.83:5.40, 3.88:3.72, 3.88:3.87, 3.88:3.89, 3.88:4.02, 3.88:4.04, 3.88:4.06, 3.88:4.19, 3.88:4.22, 3.89:3.77, 3.90:3.66, 3.94:3.66, 3.98:3.98, 4.01:3.66, 4.01:3.80, 4.02:4.07, 4.03:3.83, 4.03:4.01, 4.04:3.81, 4.04:3.88, 4.04:4.04, 4.04:4.20, 4.04:4.21, 4.06:4.01, 4.06:4.07, 4.14:3.80, 4.18:3.91, 4.20:3.77, 4.20:3.87, 4.20:3.89, 4.20:4.04, 4.20:4.19, 4.20:4.22, 4.21:3.81, 4.21:4.02, 4.21:4.06, 4.23:3.91, 4.78:4.78, 5.40:3.43, 5.40:3.48, 5.40:3.53, 5.40:3.56, 5.40:3.73, 5.40:3.75, 5.40:3.78, 5.40:3.81, 5.40:3.84, 5.40:5.40
Thumbnail	

Human Metabolome Database (HMDB)

5.2.2 1H-13C NMR Spectra



2D NMR Spectra Type	1H-13C HSQC
Spectra ID	1243
Instrument Type	Bruker
Frequency	600 MHz
Solvent	Water
pH	7.00
Shifts [ppm] (F2:F1):Intensity	3.47:71.97:0.17, 3.55:73.78:0.26, 3.66:64.07:1.00, 3.74:75.30:0.16, 3.81:62.76:0.88, 3.81:65.05:0.79, 3.83:75.16:0.25, 3.88:84.14:0.30, 4.04:76.75:0.26, 4.21:79.22:0.22, 5.40:94.80:0.68
Thumbnail	

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Sucrose | C12H22O11 - PubChem

▶ Human Metabolome Database (HMDB)

5.3 Mass Spectrometry



5.3.1 GC-MS



Showing 2 of 14 View More

Spectra ID	30233
Instrument Type	GC-EI-TOF
Ionization Mode	positive
SPLASH	splash10-0gba-0930000000-594ae5d59d217235e6c7
Top 5 Peaks	103.0 100 147.0 88.29 217.0 61.76 129.0 56.46 169.0 42.64
Thumbnail	
Notes	instrument=Pegasus III TOF-MS system, Leco; GC 6890, Agilent Technologies

▶ Human Metabolome Database (HMDB)

Spectra ID	30697
Instrument Type	GC-EI-TOF
Ionization Mode	positive
SPLASH	splash10-02ta-0932000000-8fa2c23f886fb0c63312
Top 5 Peaks	147.0 100 103.0 94.79 217.0 91.39 361.0 86.29 129.0 66.87
Thumbnail	

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Sucrose | C12H22O11 - PubChem

Notes instrument=Pegasus III TOF-MS system, Leco; GC 6890, Agilent Technologies

▶ Human Metabolome Database (HMDB)

5.3.2 MS-MS



Showing 2 of 6 View More

Spectra ID	2227157
Ionization Mode	Negative
SPLASH	splash10-000i-9500000000-292e67f588fd531ef65
Top 5 Peaks	89.02496 100 119.0361 45.60 59.01422 29.10 71.01436 28.40 113.02558 16.60
Thumbnail	

▶ Human Metabolome Database (HMDB)

Spectra ID	2227566
Ionization Mode	Negative
SPLASH	splash10-0006-2709000000-0e3c703e04384a1e3293
Top 5 Peaks	341.11018 100 179.0559 42.90 89.02527 21.10 119.03527 17.20 161.04558 9.10
Thumbnail	

https://pubchem.ncbi.nlm.nih.gov/compound/5988

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Sucrose | C12H22O11 - PubChem



▶ Human Metabolome Database (HMDB)

5.3.3 LC-MS



Showing 2 of 6 View More

Accession ID	MSBNK-RIKEN-PR100500
Authors	Matsuda F, Suzuki M, Sawada Y, Plant Science Center, RIKEN.
Instrument	UPLC Q-ToF Premier, Waters
Instrument Type	LC-ESI-QTOF
MS Level	MS2
Ionization Mode	NEGATIVE
Ionization	ESI
Collision Energy	Ramp 5-60 V
Precursor m/z	341.10841
Precursor Adduct	[M-H]-
Top 5 Peaks	341.1084 999 71.0149 800 89.0247 687 101.0245 569 179.0558 490
SPLASH	splash10-0fdx-9804000000-018a029ba3843a8db2bd
Thumbnail	
License	CC BY-SA

▶ MassBank Europe

MoNA ID	MoNA018317
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Sucrose | C12H22O11 - PubChem

MS Category	Experimental
MS Type	LC-MS
MS Level	MS2
Precursor Type	[M+Na]+
Precursor m/z	365.105438232422
Instrument	Agilent 6550 iFunnel
Instrument Type	LC-ESI-QTOF
Ionization Mode	positive
Top 5 Peaks	365.10651 24.90 272.08096 13.10
SPLASH	splash10-01b9-0049000000-aa5a4558dd60c39c28d4
Thumbnail	
Submitter	romanas chaleckis, gunma university

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

5.3.4 Other MS



Showing 2 of 6 [View More](#)

Other MS	MASS: 4955 (National Bureau of Standards EPA-NIH Mass Spectra Data Base, NSRDS- NBS-63)
----------	--

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

MoNA ID	CCMSLIB00000479739
MS Category	Experimental
MS Level	MS2
Precursor Type	[M+H]+
Precursor m/z	343.1
Instrument	Orbitrap
Ionization Mode	positive
Top 5 Peaks	127.045181 100 85.030952 95.71 145.056595 55.18 97.031975 32.84 69.035049 15
SPLASH	splash10-004s-8900000000-f71100adbafa5209fee1
Thumbnail	

<https://pubchem.ncbi.nlm.nih.gov/compound/5988>

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Sucrose | C12H22O11 - PubChem

Submitter	GNPS Team, University of California, San Diego

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

5.4 IR Spectra



IR Spectra	IR: 3335 (Coblentz Society Spectral Collection)
------------	---

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

5.4.1 FTIR Spectra



Technique	KBr (2/400)
Source of Spectrum	SPECTRA AND PROPERTIES PROVIDED BY PROFESSOR DOCTOR DIETER O. HUMMEL
Source of Sample	Commercial Cube Sugar
Copyright	Copyright © 1980, 1981-2021 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

▶ [SpectraBase](#)

Technique	KBr WAFER
Source of Sample	Merck & Company, Inc.
Copyright	Copyright © 1980, 1981-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

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[SpectraBase](#)

5.4.2 ATR-IR Spectra



Instrument Name	Bio-Rad FTS
Technique	ATR-Neat (DuraSamplIR II)
Source of Spectrum	Forensic Spectral Research
Source of Sample	USB Biochemicals, Affymetrix, Inc.
Catalog Number	Ultrapure MB Grade
Lot Number	117034
Copyright	Copyright © 2014-2021 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail



[SpectraBase](#)

Source of Sample	Aldrich
Catalog Number	247618
Copyright	Copyright © 2018-2021 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2018-2021 John Wiley & Sons, Inc. All Rights Reserved.
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► SpectraBase

5.5 Raman Spectra



Instrument Name	Thermo Nicolet FT-Raman 960
Technique	FT-Raman
Copyright	Copyright © 2003-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

► SpectraBase

Catalog Number	179949
Copyright	Copyright © 2017-2021 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2017-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

► SpectraBase

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6 Related Records



6.1 Related Compounds with Annotation



▶ PubChem

6.2 Related Compounds



Same Connectivity	180 Records
Same Stereo	20 Records
Same Isotope	151 Records
Same Parent, Connectivity	362 Records
Same Parent, Stereo	165 Records
Same Parent, Isotope	333 Records
Same Parent, Exact	146 Records
Mixtures, Components, and Neutralized Forms	364 Records
Similar Compounds	5,425 Records
Similar Conformers	92 Records

▶ PubChem

6.3 Substances



6.3.1 Related Substances



All	961 Records
Same	454 Records
Mixture	507 Records

▶ PubChem

6.3.2 Substances by Category



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Sucrose | C12H22O11 - PubChem

► PubChem

6.4 Entrez Crosslinks



PubMed	54,232 Records
Protein Structures	220 Records
Taxonomy	5 Records
OMIM	5 Records
Gene	1,455 Records

► PubChem

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Sucrose | C12H22O11 - PubChem

7 Chemical Vendors



► PubChem

8 Drug and Medication Information

8.1 FDA National Drug Code Directory

▶ [National Drug Code \(NDC\) Directory](#)

SUCROSE is an active ingredient in 35 products including: 2 TRANSFORM, ALLER-CHORD F, and ANISE PYRITE.

▶ [National Drug Code \(NDC\) Directory](#)

8.2 Clinical Trials

8.2.1 ClinicalTrials.gov

▶ [ClinicalTrials.gov](#)

8.2.2 NIPH Clinical Trials Search of Japan

<https://pubchem.ncbi.nlm.nih.gov/compound/5988>

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Sucrose | C12H22O11 - PubChem

► [NIPH Clinical Trials Search of Japan](#)

8.3 Therapeutic Uses



MEDICATION (VET): ITS ORAL USE IN ACETONEMIA OF CATTLE IS CONTROVERSIAL BUT STILL POPULAR. IT IS OFTEN USED ORALLY WITH [VINEGAR](#)...IN EMERGENCY TREATMENT OF ACUTE [UREA](#) TOXICITY IN CATTLE. DAILY ORAL USE CAN OCCASIONALLY REDUCE INCIDENCE OF BLOAT IN CATTLE ON SPRING PASTURE LOW IN CARBOHYDRATES.

Rossoff, I.S. Handbook of Veterinary Drugs. New York: Springer Publishing Company, 1974., p. 561

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

MEDICATION (VET): 20% ORAL SOLN CAUSE REFLEX CLOSURE OF ESOPHAGEAL GROOVE. ... SUGAR IS OCCASIONALLY USED...TO FACILITATE REDN OF EDEMA & EASE OF REPLACEMENT OF PROLAPSED UTERI IN COWS, EWES, BITCHES, ETC, & HAS BEEN USED LOCALLY ON WOUNDS, FOOT ROT, ETC BY LAYMEN & PROFESSIONALS.

Rossoff, I.S. Handbook of Veterinary Drugs. New York: Springer Publishing Company, 1974., p. 561

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

IV ADMIN OF HYPERTONIC SOLN OF SUCROSE HAS BEEN EMPLOYED CHIEFLY TO INITIATE OSMOTIC DIURESIS. SUCH PROCEDURE IS NOT COMPLETELY SAFE & RENAL TUBULAR DAMAGE MAY RESULT, PARTICULARLY IN PATIENTS WITH EXISTING RENAL PATHOLOGY. SAFER & MORE EFFECTIVE DIURETICS ARE AVAILABLE. /FORMER USE/

Osol, A. and J.E. Hoover, et al. (eds.). Remington's Pharmaceutical Sciences. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975., p. 1235

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

8.4 Drug Warnings



VET: ORAL ADMIN TO YOUNG ANIMALS UNABLE TO DIGEST IT WILL CAUSE OR ACCENT DIARRHEAS.

Rossoff, I.S. Handbook of Veterinary Drugs. New York: Springer Publishing Company, 1974., p. 562

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

8.5 Reported Fatal Dose



1. 1= PRACTICALLY NONTOXIC; PROBABLE ORAL LETHAL DOSE (HUMAN) ABOVE 15 G/KG, MORE THAN 1 QUART (2.2 LB) FOR 70 KG PERSON (150 LB).

Gosselin, R.E., H.C. Hodge, R.P. Smith, and M.N. Gleason. Clinical Toxicology of Commercial Products. 4th ed. Baltimore: Williams and Wilkins, 1976., p. II-151

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

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Sucrose | C12H22O11 - PubChem

9 Food Additives and Ingredients



9.1 FDA Substances Added to Food



Substance	SUCROSE
Used for (Technical Effect)	NUTRITIVE SWEETENER
	73.85
	172.810
	172.816
	172.859
Document Number (21 CFR)	172.861
	172.880
	172.884
	173.145
	184.1854

► FDA Center for Food Safety and Applied Nutrition (CFSAN)

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Sucrose | C12H22O11 - PubChem

10 Agrochemical Information



10.1 Agrochemical Category



Pesticide active substances

▶ [EU Pesticides Database](#)

10.2 EU Pesticides Data



Active Substance	sucrose
Status	Approved [Reg. (EC) No 1107/2009]
Legislation	Reg. (EU) No 916/2014

▶ [EU Pesticides Database](#)

11 Pharmacology and Biochemistry



11.1 MeSH Pharmacological Classification



Sweetening Agents

Substances that sweeten food, beverages, etc., such as sugar, saccharine or other low-calorie synthetic products. (From Random House Unabridged Dictionary, 2d ed) (See [all compounds classified as Sweetening Agents](#).)



Medical Subject Headings (MeSH)

11.2 Human Metabolite Information



11.2.1 Tissue Locations



Adipose Tissue

Bladder

Epidermis

Fibroblasts

Intestine

Kidney

Neuron

Placenta

Platelet

Prostate

Skeletal Muscle

Spleen

Testis



Human Metabolome Database (HMDB)

11.2.2 Cellular Locations



Extracellular



Human Metabolome Database (HMDB)

11.2.3 Metabolite Pathways



Galactose Metabolism

Galactosemia

Glycogen synthetase deficiency

Glycogenosis, Type III. Cori disease, Debrancher glycosinosis

Glycogenosis, Type IV. Amylopectinosis, Anderson disease

Glycogenosis, Type VI. Hers disease

Mucopolysaccharidosis VI. Sly syndrome

Starch and Sucrose Metabolism

Sucrase-isomaltase deficiency



Human Metabolome Database (HMDB)

11.3 Biochemical Reactions



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► [Rhea - Annotated Reactions Database](#)

► [PubChem](#)

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12 Use and Manufacturing



12.1 Uses



EPA CPDat Chemical and Product Categories

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

▶ EPA Chemical and Products Database (CPDat)

Sources/Uses

Obtained from cane sugar, sugar beet, and sorghum; Used as a sweetener; [ChemIDplus]

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

For Sucrose (USEPA/OPP Pesticide Code: 000023) there are 0 labels match. /SRP: Not registered for current use in the U.S., but approved pesticide uses may change periodically and so federal, state and local authorities must be consulted for currently approved uses./ U.S. Environmental Protection Agency/Office of Pesticide Program's Chemical Ingredients Database on Sucrose (57-50-1). Available from, as of Sept 8, 2000: <https://npispublic.ceris.purdue.edu/ppis/>

▶ Hazardous Substances Data Bank (HSDB)

FLAVOR BLENDER, ACCENTUATOR, MODIFIER & DISPERSING AGENT, SWEETENING, TEXTURE & BODYING AGENT FOR FOODS & BEVERAGES; RAW MATERIAL FOR NUMEROUS ORG CHEM & YEAST PRODN; LUBRICANT IN FOODS

SRI

▶ Hazardous Substances Data Bank (HSDB)

Sweetener in foods and soft drinks, manufacture of syrups, source of invert sugar, confectionary, preserves and jams, demulcent, pharmaceutical products, caramel, chemical intermediate for detergents, emulsifying agents, and other sucrose derivatives.

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 1058

▶ Hazardous Substances Data Bank (HSDB)

Sweetening agent and food. Starting material in fermentative prodn of ethanol, butanol, glycerol, citric and levulinic acids. Used in pharmaceuticals as a flavor, as a preservative, as antioxidant (in form of invert sugar), as demulcent, as substitute for glycerol, as granulation agent and excipient for tablets, as coating for tablets. In plastics and cellulose industry, in rigid polyurethane foams, manuf of ink and of transparent soaps.

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1518

▶ Hazardous Substances Data Bank (HSDB)

For more Uses (Complete) data for SUCROSE (9 total), please visit the [HSDB record page](#).

▶ Hazardous Substances Data Bank (HSDB)

12.1.1 Use Classification



EPA Safer Chemical Functional Use Classes -> Processing Aids and Additives

▶ EPA Safer Choice

<https://pubchem.ncbi.nlm.nih.gov/compound/5988>

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Sucrose | C12H22O11 - PubChem

Safer Chemical Classes ->  Green circle - The chemical has been verified to be of low concern

▶ [EPA Safer Choice](#)

Agrochemicals -> Pesticides

▶ [EU Pesticides Database](#)

Cosmetics -> Humectant; Skin conditioning; Soothing

513 | *EUCOSMETICS* | *Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006)* | [DOI:10.5281/zenodo.2624118](#)

▶ [NORMAN Suspect List Exchange](#)

12.1.2 Industry Uses



Adhesives and sealant chemicals
Intermediates

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

▶ [EPA Chemicals under the TSCA](#)

12.1.3 Consumer Uses



Cleaning and furnishing care products
Furniture and furnishings not covered elsewhere

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

▶ [EPA Chemicals under the TSCA](#)

12.1.4 Household Products



Household & Commercial/Institutional Products

Information on 73 consumer products that contain Sucrose in the following categories is provided:

- Inside the Home
 - Personal Care
 - Pesticides
 - Pet Care
- ▶ [Consumer Product Information Database \(CPID\)](#)

12.2 Methods of Manufacturing



Obtained from sugar cane (*Saccharum officinarum* L, Gramineae) and sugar beet (*Beta vulgaris* L, Chenopodiaceae). Sugar cane contains from 15-20% and sugar beet form 10-17% sucrose. Structure: Avery et al, J Chem Soc 1927, 2308; Beevers, Cochrane, Proc Roy Soc 190a, 257 (1947).

Budavari, S. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1518

▶ [Hazardous Substances Data Bank \(HSDb\)](#)

By crushing and extraction of sugarcane (*Saccharum officinarum*) with [water](#) or extraction of the sugar beet (*Beta vulgaris*) with [water](#), evaporating, and purifying with lime, [carbon](#), and various liquids. Also obtainable from sorghum by conventional methods.

Lewis, R.J., Sr (Ed.). *Hawley's Condensed Chemical Dictionary*. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 1057

▶ [Hazardous Substances Data Bank \(HSDb\)](#)

Sucrose is extracted commercially from sugar maple

KIRK-OTHMER CONDENSED ENCYC CHEM TECH 1985 p.1118

▶ [Hazardous Substances Data Bank \(HSDb\)](#)

<https://pubchem.ncbi.nlm.nih.gov/compound/5988>

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Sucrose | C12H22O11 - PubChem

12.3 Formulations/Preparations



USEPA/OPP Pesticide Code 000023; Trade Names: None.
U.S. Environmental Protection Agency/Office of Pesticide Program's Chemical Ingredients Database on Sucrose (57-50-1). Available from, as of Sept 8, 2000: <https://npirspublic.ceris.purdue.edu/ppis/>
▶ [Hazardous Substances Data Bank \(HSDb\)](#)

Grade: Reagent, USP, technical, refined.
Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 1057
▶ [Hazardous Substances Data Bank \(HSDb\)](#)

Also sold as syrup .. liquid sugar
Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA4 (85) 65
▶ [Hazardous Substances Data Bank \(HSDb\)](#)

12.4 Consumption Patterns



(DELIVERIES OF REFINED SUGAR): 35% WAS CONSUMED DIRECTLY FOR SWEETENING FOODS & BEVERAGES; THE REMAINING 65% WAS USED INDUSTRIALLY IN BEVERAGES (22%); IN BAKERY & CEREAL PRODUCTS (12%); IN CONFECTIONS (9%); IN CANNED, BOTTLED, & FROZEN FOODS (6%); IN ICE CREAM & DAIRY PRODUCTS (5%); IN MISC FOODS (5%); & IN NON-FOOD & UNSPECIFIED USES (6%) (1976)
SRI
▶ [Hazardous Substances Data Bank \(HSDb\)](#)

12.5 U.S. Production



Aggregated Product Volume (EPA CDR 2016)
1,000,000,000 - 5,000,000,000 lb
<https://www.epa.gov/chemical-data-reporting>
▶ [EPA Chemicals under the TSCA](#)

(1972) 5.01X10+13 G (CANE & BEET SUGAR)
SRI
▶ [Hazardous Substances Data Bank \(HSDb\)](#)

(1975) 5.19X10+13 G (CANE AND BEET SUGAR)
SRI
▶ [Hazardous Substances Data Bank \(HSDb\)](#)

12.6 U.S. Imports



(1972) 4.77X10+12 G (CANE/BEET SUGAR & SYRUP)
SRI
▶ [Hazardous Substances Data Bank \(HSDb\)](#)

(1975) 3.62X10+12 G
SRI
▶ [Hazardous Substances Data Bank \(HSDb\)](#)

(1984) 3.28X10+12 g /Cane or beet sugars, syrups, molasses, NSPF (Raw Value)/
BUREAU OF THE CENSUS. U.S. IMPORTS FOR CONSUMPTION AND GENERAL IMPORTS 1984 p.1-41
▶ [Hazardous Substances Data Bank \(HSDb\)](#)

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Sucrose | C12H22O11 - PubChem

12.7 U.S. Exports



(1972) 7.06X10+8 G (CANE/BEET, RAW & REFINED)

SRI

▶ [Hazardous Substances Data Bank \(HSDb\)](#)

(1975) 1.87X10+11 G

SRI

▶ [Hazardous Substances Data Bank \(HSDb\)](#)

(1984) 2.79X10+10 g /Sugar cane, beet, crystalline structure or dry amorphous form, refined/

BUREAU OF THE CENSUS. U.S. EXPORTS, SCHEDULE E, 1984 p.2-25

▶ [Hazardous Substances Data Bank \(HSDb\)](#)

12.8 General Manufacturing Information



Industry Processing Sectors

Furniture and related product manufacturing
Wood product manufacturing

▶ [EPA Chemicals under the TSCA](#)

EPA TSCA Commercial Activity Status

.alpha.-D-Glucopyranoside, .beta.-D-fructofuranosyl: ACTIVE

<https://www.epa.gov/tsc-inventory>

▶ [EPA Chemicals under the TSCA](#)

CARBOHYDRATE (QV) PRODUCT OF PHOTOSYNTHESIS COMPRISED OF 1, 2, OR MORE SACCHAROSE GROUPS. ... SUGAR IS IMPORTANT SOURCE OF METABOLIC ENERGY IN FOODS, & ITS FORMATION IN PLANTS IS ESSENTIAL FACTOR IN LIFE PROCESS.

Hawley, G.G. The Condensed Chemical Dictionary. 9th ed. New York: Van Nostrand Reinhold Co., 1977., p. 823

▶ [Hazardous Substances Data Bank \(HSDb\)](#)

Sucrose is the most important industrial sugar

KIRK-OTHMER CONDENSED ENCYC CHEM TECH 1985 p.202

▶ [Hazardous Substances Data Bank \(HSDb\)](#)

Sucrose was first synthesized enzymatically in the laboratory from potassium D-glucosyl-1-phosphate and [D-fructose](#). The first chemical synthesis was accomplished by reaction of [3,4,6-tri-O-acetyl-1,2-anhydro-alpha-D-glucopyranose](#) with [1,3,4,6-tetra-O-acetyl-D-fructofuranose](#)

Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984., p. V21 865

▶ [Hazardous Substances Data Bank \(HSDb\)](#)

Traditionally, the standard /sweetening agent/ is sucrose, both in terms of quality of taste and taste profile

Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984., p. V22 448

▶ [Hazardous Substances Data Bank \(HSDb\)](#)

For more General Manufacturing Information (Complete) data for SUCROSE (6 total), please visit the [HSDb record page](#).

▶ [Hazardous Substances Data Bank \(HSDb\)](#)

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Sucrose | C12H22O11 - PubChem

13 Identification



13.1 Analytic Laboratory Methods



SUGARS & SUGAR PRODUCTS BY POLARIMETRIC METHODS.
Association of Official Analytical Chemists. Official Methods of Analysis. 10th ed. and supplements. Washington, DC: Association of Official Analytical Chemists, 1965. New editions through 13th ed. plus supplements, 1982., p. 12/567 31.020

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

DETERMINATION IN FOODSTUFF BY SPECTROPHOTOMETRY @ 340, 334, OR 365 NM.
Bergmeyer, H.W. (ed.). Methods of Enzymatic Analysis. 2nd English ed. New York City: Academic Press, 1974., p. 1176

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

14 Safety and Hazards



14.1 Hazards Identification

GHS Hazard Statements	Not Classified
	Reported as not meeting GHS hazard criteria by 410 of 425 companies provided GHS information). For more detailed information, please visit ECHA C&L website .

European Chemicals Agency (ECHA)

14.1.2 EPA Safer Chemical



Chemical: Sucrose



Green circle - The chemical has been verified to be of low concern based on experimental and modeled data.

EPA Safer Choice

14.1.3 Health Hazards



None (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

14.1.4 Fire Hazards



Special Hazards of Combustion Products: Irritating fumes may form in fires. Behavior in Fire: Melts and chars (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

Combustible. Finely dispersed particles form explosive mixtures in air.

ILO International Chemical Safety Cards (ICSC)

14.1.5 Hazards Summary



May cause mechanical irritation; [LCSC]

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

14.2 Safety and Hazard Properties



14.2.1 Flammable Limits



Flammability

Noncombustible Solid, but fine airborne dust may explode.

The National Institute for Occupational Safety and Health (NIOSH)

14.2.2 Lower Explosive Limit (LEL)



0.045 g/L (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.

<https://pubchem.ncbi.nlm.nih.gov/compound/5988>

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▶ CAMEO Chemicals

0.045 g/L

▶ Occupational Safety and Health Administration (OSHA)

14.2.3 Physical Dangers



Dust explosion possible if in powder or granular form, mixed with air.

▶ ILO International Chemical Safety Cards (ICSC)

14.2.4 OSHA Standards



Permissible Exposure Limit: Table Z-1 8-hr Time Weighted Avg: 15 mg/cu m. /Total dust/

29 CFR 1910.1000 (7/1/2000)

▶ Hazardous Substances Data Bank (HSDb)

Permissible Exposure Limit: Table Z-1 8-hr Time Weighted Avg: 5 mg/cu m. /Respirable fraction/

29 CFR 1910.1000 (7/1/2000)

▶ Hazardous Substances Data Bank (HSDb)

14.2.5 NIOSH Recommendations



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

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 288

▶ Hazardous Substances Data Bank (HSDb)

Recommended Exposure Limit: 10 Hr Time-Weighted Avg: 5 mg/cu m (resp).

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 288

▶ Hazardous Substances Data Bank (HSDb)

14.3 First Aid Measures



14.3.1 First Aid



EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with [water](#) or [normal saline](#) solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician. If symptoms (such as redness or irritation) develop, immediately transport the victim to a hospital. SKIN: IMMEDIATELY flood affected skin with [water](#) while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and [water](#). If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment. INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing. INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of [water](#) to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport the victim to a hospital. (NTP, 1992)

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

▶ CAMEO Chemicals

(See 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.

Breathing: Fresh air

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

14.3.2 Inhalation First Aid



<https://pubchem.ncbi.nlm.nih.gov/compound/5988>

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Fresh air, rest.

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

14.3.3 Skin First Aid



Rinse skin with plenty of [water](#) or shower.

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

14.3.4 Eye First Aid



First rinse with plenty of [water](#) for several minutes (remove contact lenses if easily possible), then refer for medical attention.

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

14.4 Fire Fighting



Fire Extinguishing Agents: [Water](#) (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](#)

Use [water](#) spray, powder, alcohol-resistant foam, [carbon dioxide](#). In case of fire: keep drums, etc., cool by spraying with [water](#).

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

14.4.1 Fire Fighting Procedures



Water

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 \(HSDb\)](#)

14.4.2 Firefighting Hazards



Irritating fumes may form in fires.

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 \(HSDb\)](#)

14.5 Accidental Release Measures



14.5.1 Spillage Disposal



Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting.

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

14.5.2 Disposal Methods



SRP: At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices.

▶ [Hazardous Substances Data Bank \(HSDb\)](#)

14.6 Handling and Storage



<https://pubchem.ncbi.nlm.nih.gov/compound/5988>

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14.6.1 Nonfire Spill Response



SMALL SPILLS AND LEAKAGE: If you spill this chemical, you should dampen the solid spill material with [water](#), then transfer the dampened material to a suitable container. Use absorbent paper dampened with [water](#) to pick up any remaining material. Seal your contaminated clothing and the absorbent paper in a vapor-tight plastic bag for eventual disposal. Wash all contaminated surfaces with a soap and [water](#) solution. Do not reenter the contaminated area until the Safety Officer (or other responsible person) has verified that the area has been properly cleaned. STORAGE PRECAUTIONS: You should store this material under ambient temperatures. (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](#)

14.6.2 Safe Storage



Separated from strong oxidants.

► [ILO International Chemical Safety Cards \(ICSC\)](#)

14.7 Exposure Control and Personal Protection



14.7.1 Recommended Exposure Limit (REL)



REL-TWA (Time Weighted Average)

10 mg/m³ (total), 5 mg/m³ (resp)

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

TWA 10 mg/m³ (total) TWA 5 mg/m³ (resp)

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

14.7.2 Permissible Exposure Limit (PEL)



15.0 [mg/m³](total dust), 5 mg/m³(respirable fraction)

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

PEL-TWA (8-Hour Time Weighted Average)

15 mg/m³ (total dust), 5 mg/m³ (respirable fraction)

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

TWA 15 mg/m³ (total) TWA 5 mg/m³ (resp)

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

14.7.3 Immediately Dangerous to Life or Health (IDLH)



N.D.

See: [IDLH INDEX](#)

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

14.7.4 Threshold Limit Values (TLV)



10.0 [mg/m³]

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

8 hr Time Weighted Avg (TWA): 10 mg/cu m

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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. 53

[▶ 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 \(HSDb\)](#)

A4: Not classifiable as a human carcinogen.

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. 53

[▶ Hazardous Substances Data Bank \(HSDb\)](#)

10 mg/m3, as TWA; A4 (not classifiable as a human carcinogen)

[▶ ILO International Chemical Safety Cards \(ICSC\)](#)

TLV-TWA (Time Weighted Average)

10 mg/m³ [1992]

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

14.7.5 Effects of Short Term Exposure



May cause mechanical irritation.

[▶ ILO International Chemical Safety Cards \(ICSC\)](#)

14.7.6 Effects of Long Term Exposure



The substance may have effects on the teeth. This may result in dental caries. Repeated or prolonged contact with skin may cause dermatitis.

[▶ ILO International Chemical Safety Cards \(ICSC\)](#)

14.7.7 Allowable Tolerances



Residues of sucrose are exempted from the requirement of a tolerance when used as a solid diluent, carrier or safener in accordance with good agricultural practices as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops or to raw agricultural commodities after harvest.

40 CFR 180.1001(c) (7/1/2000)

[▶ Hazardous Substances Data Bank \(HSDb\)](#)

Sucrose is exempted from the requirement of a tolerance when used as a solid diluent or carrier in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to animals.

40 CFR 180.1001(e) (7/1/2000)

[▶ Hazardous Substances Data Bank \(HSDb\)](#)

14.7.8 Personal Protective Equipment (PPE)



Excerpt from NIOSH Pocket Guide for Sucrose: Skin: No recommendation is made specifying the need for personal protective equipment for the body. Eyes: No recommendation is made specifying the need for eye protection. Wash skin: No recommendation is made specifying the need for washing the substance from the skin (either immediately or at the end of the work shift). Remove: No recommendation is made specifying the need for removing clothing that becomes wet or contaminated. Change: No recommendation is made specifying the need for the worker to change clothing after the workshift. (NIOSH, 2022)

[▶ CAMEO Chemicals](#)

/NIOSH approved respirator/ and goggles or face shield.

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 \(HSDb\)](#)

<https://pubchem.ncbi.nlm.nih.gov/compound/5988>

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(See protection codes)

Skin: No recommendation

Eyes: No recommendation

Wash skin: No recommendation

Remove: No recommendation

Change: No recommendation

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

14.7.9 Respirator Recommendations

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

Important additional information about respirator selection

14.7.10 Fire Prevention

NO open flames. Closed system, dust explosion-proof electrical equipment and lighting. Prevent deposition of dust.

► ILO International Chemical Safety Cards (ICSC)

14.7.11 Inhalation Prevention

Use local exhaust or breathing protection.

► ILO International Chemical Safety Cards (ICSC)

14.7.12 Skin Prevention

Protective gloves.

► ILO International Chemical Safety Cards (ICSC)

14.7.13 Eye Prevention

Wear safety goggles.

► ILO International Chemical Safety Cards (ICSC)

14.8 Stability and Reactivity

► ILO International Chemical Safety Cards (ICSC)

14.8.1 Air and Water Reactions

Water soluble. Sugar dust explosion is possibility.

► CAMEO Chemicals

14.8.2 Reactive Group

Alcohols and Polyols

► CAMEO Chemicals

14.8.3 Reactivity Profile

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SUCROSE is a reducing agent. Can react explosively with oxidizing agents such as chlorates and perchlorates. Is hydrolyzed by dilute acids and by invertase (a yeast enzyme) (NTP, 1992). Chars rapidly and exothermically when mixed with concentrated [sulfuric acid](#).
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](#)

14.8.4 Hazardous Reactivities and Incompatibilities



Oxidizers, [sulfuric acid](#), [nitric acid](#).
NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 288
▶ [Hazardous Substances Data Bank \(HSDb\)](#)

14.9 Regulatory Information



14.9.1 FIFRA Requirements



Residues of sucrose are exempted from the requirement of a tolerance when used as a solid diluent, carrier or safener in accordance with good agricultural practices as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops or to raw agricultural commodities after harvest.
40 CFR 180.1001(c) (7/1/2000)
▶ [Hazardous Substances Data Bank \(HSDb\)](#)

Sucrose is exempted from the requirement of a tolerance when used as a solid diluent or carrier in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to animals.
40 CFR 180.1001(e) (7/1/2000)
▶ [Hazardous Substances Data Bank \(HSDb\)](#)

14.9.2 FDA Requirements



Substance added directly to human food affirmed as generally recognized as safe (GRAS).
21 CFR 184.1854 (4/1/2000)
▶ [Hazardous Substances Data Bank \(HSDb\)](#)

14.10 Other Safety Information



14.10.1 Special Reports



INFORMATICS INC; SCIENTIFIC LITERATURE REVIEWS ON GENERALLY RECOGNIZED AS SAFE (GRAS) FOOD INGREDIENTS: SUCROSE; US NTIS PB REPORT PB-228 548, 202 PP. (1973). LITERATURE REVIEW OF SUCROSE AND ITS USE IN FOOD PRODUCTS.
▶ [Hazardous Substances Data Bank \(HSDb\)](#)

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Sucrose | C12H22O11 - PubChem

15 Toxicity

?

15.1 Toxicological Information

?

15.1.1 NIOSH Toxicity Data

?

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

15.1.2 Evidence for Carcinogenicity

?

A4: Not classifiable as a human carcinogen.
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. 53
▶ Hazardous Substances Data Bank (HSDb)

15.1.3 Exposure Routes

?

The substance can be absorbed into the body by inhalation and by ingestion.
▶ ILO International Chemical Safety Cards (ICSC)

inhalation, skin and/or eye contact
▶ The National Institute for Occupational Safety and Health (NIOSH)

15.1.4 Symptoms

?

irritation eyes, skin, upper respiratory system; cough
▶ The National Institute for Occupational Safety and Health (NIOSH)

15.1.5 Inhalation Symptoms

?

Cough.
▶ ILO International Chemical Safety Cards (ICSC)

15.1.6 Skin Symptoms

?

Redness. Roughness.

► ILO International Chemical Safety Cards (ICSC)

15.1.7 Eye Symptoms

Redness.

► ILO International Chemical Safety Cards (ICSC)

15.1.8 Target Organs

Eyes, respiratory system

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

15.1.9 Adverse Effects

ACGIH Carcinogen - Not Classifiable.

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

15.1.10 Acute Effects

► ChemIDplus

15.1.11 Human Toxicity Excerpts

Liquid medicines, particularly those intended for children, often formulated as syrups, usually based on sucrose. Total sugar content may be up to 80% (w/v). Complicated diabetes management. Increased dental caries especially in chronically sick children (eg, asthmatics or epileptics) who frequently take liquid medicine.

Ellenhorn, M.J. and D.G. Barceloux. *Medical Toxicology - Diagnosis and Treatment of Human Poisoning*. New York, NY: Elsevier Science Publishing Co., Inc. 1988. p. 527

► Hazardous Substances Data Bank (HSDB)

Sucrose is reported to be capable of producing dermatoses in bakers, candy makers, and related occupations. It is well established that uncontrolled [glucose](#) conc in maternal blood are associated with elevated embryonic and fetal death and increased neonatal morbidity and mortality.

American Conference of Governmental Industrial Hygienists, Inc. *Documentation of the Threshold Limit Values and Biological Exposure Indices*. 6th ed. Volumes I, II, III. Cincinnati, OH: ACGIH, 1991. p. 1450

► Hazardous Substances Data Bank (HSDB)

15.1.12 Non-Human Toxicity Excerpts

EVIDENCE EXISTS THAT HIGHLY CONCN SOLN ARE LETHAL TO NEMATODES IN SOIL.

<https://pubchem.ncbi.nlm.nih.gov/compound/5988>

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Rossoff, I.S. *Handbook of Veterinary Drugs*. New York: Springer Publishing Company, 1974., p. 562

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

DIFFUSE PATHOLOGICAL CHANGES /IN POISONED ANIMALS/ INCL SHRINKAGE, SWELLING & NECROSIS OF RENAL TUBULAR EPITHELIUM, ARTERIOLITIS, MILD HEPATITIS, MYOCARDITIS, CONGESTIVE ENCEPHALITIS & SOME ADRENAL HYPERTROPHY.

Gosselin, R.E., R.P. Smith, H.C. Hodge. *Clinical Toxicology of Commercial Products*. 5th ed. Baltimore: Williams and Wilkins, 1984., p. II-227

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

SUCROSE HAS SHOWN NO TOXICITY TO CORNEAS OF RABBITS WHEN APPLIED FOR 3 TO 7 HR IN NEUTRAL AQ SOLN...

Grant, W. M. *Toxicology of the Eye*. 2nd ed. Springfield, Illinois: Charles C. Thomas, 1974., p. 949

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

...CANE SUGAR...OBSERVED TO CAUSE DIARRHEA, COLIC, INFLAMMATION OF KIDNEYS &...PETECHIAL HEMORRHAGES IN SPINAL DURA MATER OF HORSES.

Clarke, E.G., and M. L. Clarke. *Veterinary Toxicology*. Baltimore, Maryland: The Williams and Wilkins Company, 1975., p. 284

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

For more Non-Human Toxicity Excerpts (Complete) data for SUCROSE (14 total), please visit the [HSDB record page](#).

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

15.1.13 Non-Human Toxicity Values



LD50 Rat oral 29,700 mg/kg

Sax, N.I. *Dangerous Properties of Industrial Materials*. 6th ed. New York, NY: Van Nostrand Reinhold, 1984., p. 2478

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

15.1.14 Populations at Special Risk



Patients with severe malabsorption secondary to disease or resection ... may have deficiency of other disaccharidases and large amounts of sucrose should be avoided /in enteral formulations/.

American Medical Association, Council on Drugs. *AMA Drug Evaluations Annual 1994*. Chicago, IL: American Medical Association, 1994., p. 2195

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

15.2 Ecological Information



15.2.1 Natural Pollution Sources



Occurs in low percentages in honey and maple sap

Lewis, R.J., Sr (Ed.). *Hawley's Condensed Chemical Dictionary*. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 1057

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

Sugar cane contains from 15-20% and sugar beet from 10-17% sucrose

Budavari, S. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1517

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

The quantity of sucrose synthesized by all plants on earth is estimated to be 150X10+9 t/a.

Gerhartz, W. (exec ed.). *Ullmann's Encyclopedia of Industrial Chemistry*. 5th ed. Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA 5 (86) 83

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

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16 Associated Disorders and Diseases



▶ Comparative Toxicogenomics Database (CTD)

Disease	References
Colorectal cancer	PubMed: 7482520, 19006102, 23940645, 24424155, 20156336, 19678709, 22148915, 25105552, 21773981, 25037050, 27015276, 27107423, 27275383, 28587349 Silke Matsik, Caroline Ivanne Le Roy, Gerhard Liebisch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. Trends in Food Science & Technology. Vol. 57, Part B, Nov. 2016, p.244-255: http://www.sciencedirect.com/science/article/pii/S0924224416301984
Crohn's disease	PubMed: 16440420, 11418788, 8723414, 19491857, 17269711, 23516449, 23867873, 24811995, 25598765, 26806034, 26848182, 27609529, 28842642
Ulcerative colitis	PubMed: 21059682, 1740537, 17269711, 17314143, 21761941, 23516449, 23867873, 24811995, 25598765, 26806034, 26848182, 27609529, 28842642
Sepsis	PubMed: 9141546, 19034423, 28701177
Attachment loss	PubMed: 31026179
Periodontal Probing Depth	PubMed: 31026179
Lung Cancer	PubMed: 22157537, 18953024, 25961003
Autosomal dominant polycystic kidney disease	PubMed: 18215696, 21389975
Eosinophilic esophagitis	Mordechai, Hien, and David S. Wishart

▶ Human Metabolome Database (HMDB)

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17 Literature



17.1 Coronavirus Studies



► PubChem

17.2 NLM Curated PubMed Citations



► PubChem

17.3 Springer Nature References



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► Springer Nature

17.4 Thieme References



► Thieme Chemistry

17.5 Depositor Provided PubMed Citations



► PubChem

17.6 Synthesis References



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17.7 Metabolite References



▶ Human Metabolome Database (HMDB)

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17.9 Chemical Co-Occurrences in Literature



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17.10 Chemical-Gene Co-Occurrences in Literature



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17.11 Chemical-Disease Co-Occurrences in Literature



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18 Patents



18.1 Depositor-Supplied Patent Identifiers



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18.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

<https://patentscope.wipo.int/search/en/result.jsf?inchikey=CZMRCDWAGMRECN-UGDNZRGBSA-N>

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19 Interactions and Pathways



19.1 Protein Bound 3D Structures



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19.2 Chemical-Target Interactions



► [Comparative Toxicogenomics Database \(CTD\)](#)

► [DrugBank](#)

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► Therapeutic Target Database (TTD)

19.3 Pathways



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20 Biological Test Results



20.1 BioAssay Results



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21 Taxonomy



Sucrose is a metabolite found in or produced by [Escherichia coli](#) (strain K12, MG1655).

► [E. coli Metabolome Database \(ECMDB\)](#)

WormJam Metabolites Local CSV for MetFrag | [DOI:10.5281/zenodo.3403364](#)
WormJam: A consensus C. elegans Metabolic Reconstruction and Metabolomics Community and Workshop Series, Worm, 6:2, e1373939, [DOI:10.1080/21624054.2017.1373939](#)

► [ECI Group, LCSB, University of Luxembourg](#)

Zebrafish Pathway Metabolite MetFrag Local CSV (Beta) | [DOI:10.5281/zenodo.3457553](#)

► [ECI Group, LCSB, University of Luxembourg](#)

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The LOTUS Initiative for Open Natural Products Research: frozen dataset union wikidata (with metadata) | DOI:10.5281/zenodo.5794106

► [LOTUS - the natural products occurrence database](#)

Sucrose is a metabolite found in or produced by [Saccharomyces cerevisiae](#).

► [Yeast Metabolome Database \(YMDB\)](#)

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22 Classification



22.1 MeSH Tree



► Medical Subject Headings (MeSH)

22.2 NCI Thesaurus Tree



► NCI Thesaurus (NCIt)

22.3 ChEBI Ontology



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► ChEBI

22.4 KEGG: Metabolite



► KEGG

22.5 KEGG: Drug



► KEGG

22.6 KEGG: JP15



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▶ KEGG

22.7 KEGG: Risk Category of Japanese OTC Drugs



▶ KEGG

22.8 EPA Safer Choice



▶ EPA Safer Choice

22.9 ChemIDplus



22.10 CAMEO Chemicals

▶ ChemIDplus



22.11 CHEMBL Target Tree

▶ CAMEO Chemicals



▶ ChEMBL

22.12 UN GHS Classification

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► UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

22.13 EPA CPDat Classification



► EPA Chemical and Products Database (CPDat)

22.14 NORMAN Suspect List Exchange Classification



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▶ NORMAN Suspect List Exchange

22.15 CCSBase Classification



▶ CCSbase

22.16 EPA DSSTox Classification



▶ EPA DSSTox

22.17 Consumer Product Information Database Classification



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▶ Consumer Product Information Database (CPID)

22.18 LOTUS Tree



▶ LOTUS - the natural products occurrence database

22.19 FDA Drug Type and Pharmacologic Classification



▶ National Drug Code (NDC) Directory

22.20 EPA Substance Registry Services Tree



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<https://www.ncbi.nlm.nih.gov/mesh/68013395>

MeSH Tree
<http://www.nlm.nih.gov/mesh/meshhome.html>

Sweetening Agents
<https://www.ncbi.nlm.nih.gov/mesh/68013549>

48. **KEGG**

LICENSE
Academic users may freely use the KEGG website. Non-academic use of KEGG generally requires a commercial license
<https://www.kegg.jp/kegg/legal.html>

Compounds with biological roles
http://www.genome.jp/kegg-bin/get_htext?br08001.keg

Therapeutic category of drugs in Japan
http://www.genome.jp/kegg-bin/get_htext?br08301.keg

Drugs listed in the Japanese Pharmacopoeia
http://www.genome.jp/kegg-bin/get_htext?br08311.keg

Risk category of Japanese OTC drugs
http://www.genome.jp/kegg-bin/get_htext?br08312.keg

49. **UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)**

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

50. **ChEMBL**

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Access to the web interface of ChEMBL is made under the EBI's Terms of Use (<http://www.ebi.ac.uk/Information/termsfuse.html>). The ChEMBL data is made available on a Creative Commons Attribution-Share Alike 3.0 Unported License (<http://creativecommons.org/licenses/by-sa/3.0/>).
<http://www.ebi.ac.uk/Information/termsfuse.html>

ChEMBL Protein Target Tree
<https://www.ebi.ac.uk/chembl/g/#browse/targets>

51. **EPA Substance Registry Services**

LICENSE

<https://pubchem.ncbi.nlm.nih.gov/compound/5988>

11/13/22, 5:40 PM

Sucrose | C12H22O11 - PubChem

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

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

52. **PATENTSCOPE (WIPO)**

SID 403029430
<https://pubchem.ncbi.nlm.nih.gov/substance/403029430>