

COMPOUND SUMMARY

Trehalose dihydrate



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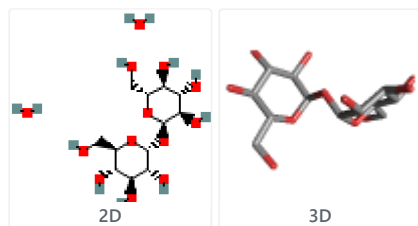
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PubChem CID: 181978

Structure:

[Find Similar Structures](#)Molecular Formula: C₁₂H₂₆O₁₃

Chemical Names:

6138-23-4
D-(+)-Trehalose dihydrate
Trehalose dihydrate
a,a-Trehalose
UNII-7YIN7J07X4[More...](#)

Molecular Weight: 378.33 g/mol

Dates:

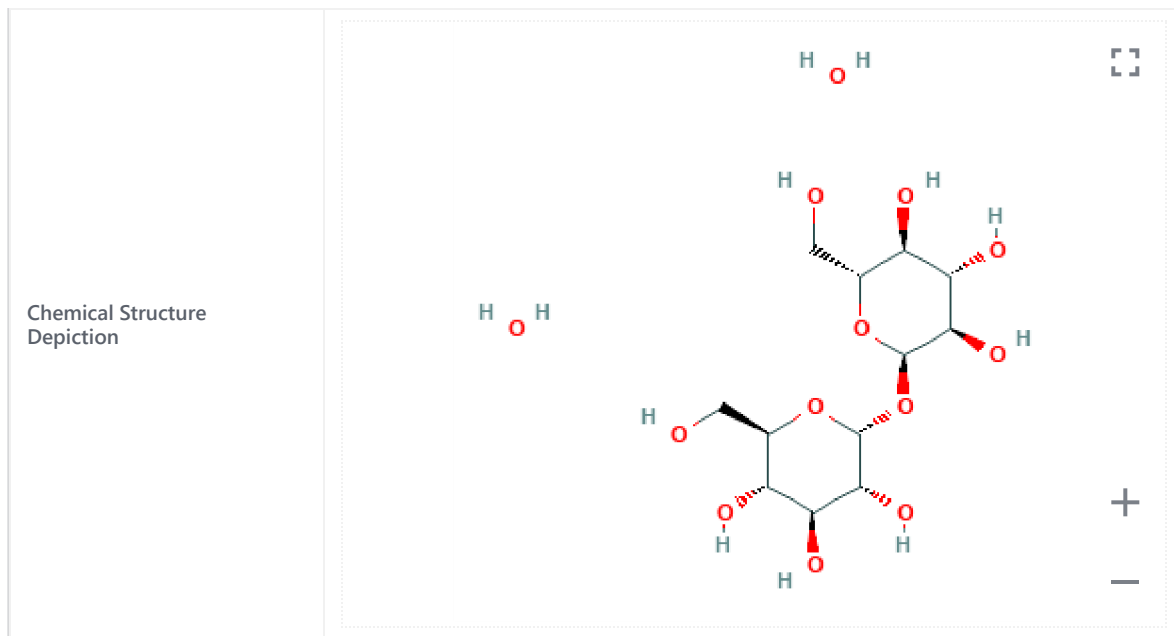
Modify: 2019-08-24
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1 Structures



1.1 2D Structure

[Find Similar Structures](#) [Get Image](#) [Download](#)



▶ from PubChem

1.2 3D Conformer



3D Conformer of Parent

▶ from PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

(2*R*,3*S*,4*S*,5*R*,6*R*)-2-(hydroxymethyl)-6-[(2*R*,3*R*,4*S*,5*S*,6*R*)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-3,4,5-triol;dihydrate

▶ from PubChem

2.1.2 InChI

InChI=1S/C12H22O11.2H2O/c13-1-3-5(15)7(17)9(19)11(21-3)23-12-10(20)8(18)6(16)4(2-14)22-12;;/h3-20H,1-2H2;2*1H2/t3-,4-,5-,6-,7+,8+,9-,10-,11-,12-;;/m1../s1

▶ from PubChem

2.1.3 InChI Key

DPVHGFAJLZWDOC-PVXXTIHASA-N

▶ from PubChem

2.1.4 Canonical SMILES

C(C1C(C(C(C(O1)OC2C(C(C(C(O2)CO)O)O)O)O)O)O)O.O.O

▶ from PubChem

2.1.5 Isomeric SMILES

C([C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)O[C@@H]2[C@@H]([C@H]([C@@H]([C@H](O2)CO)O)O)O)O)O)O.O.O

▶ from PubChem

2.2 Molecular Formula



C₁₂H₂₆O₁₃

▶ from PubChem

2.3 Other Identifiers



2.3.1 CAS



6138-23-4

▶ from ChemIDplus; EPA DSSTox; European Chemicals Agency (ECHA)

Other CAS

219843-81-9

▶ from ChemIDplus

2.3.2 European Community (EC) Number



612-140-5

▶ from European Chemicals Agency (ECHA)

2.3.3 FEMA Number



4600

▶ from Flavor and Extract Manufacturers Association (FEMA)

2.3.4 UNII



7YIN7J07X4

▶ from FDA/SPL Indexing Data

2.3.5 Wikipedia



Trehalose dihydrate

▶ from Wikipedia

2.4 Synonyms



2.4.1 Depositor-Supplied Synonyms



6138-23-4	AK117470
D-(+)-Trehalose dihydrate	alp,alp.-Trehalose
Trehalose dihydrate	(2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)tetrahydropyran-3,4,5-triol
a,a-Trehalose	dextro-trehalose dihydrate
UNII-7YIN7J07X4	a,a-D-Trehalose dihydrate
D-Trehalose dihydrate	99-20-7 (anhydrous)
alpha,alpha-Trehalose dihydrate	DSSTox_CID_27948
MFCD00071594	DSSTox_RID_82700
7YIN7J07X4	DSSTox_GSID_47972
D(+)-Trehalose dihydrate	SCHEMBL166078
D(+)-Trehalose dihydrate, 99%	AC1L4A22
d-trehalose-dihyd	CHEMBL3188936
Mycose,1-O-alpha-D-glucopyranosyl-alpha-D-glucopyranoside	

▶ from PubChem

3 Chemical and Physical Properties



3.1 Computed Properties



Property Name	Property Value
Molecular Weight	378.33 g/mol
Hydrogen Bond Donor Count	10

Property Name	Property Value
Hydrogen Bond Acceptor Count	13
Rotatable Bond Count	4
Exact Mass	378.137341 g/mol
Monoisotopic Mass	378.137341 g/mol
Topological Polar Surface Area	192 A ²
Heavy Atom Count	25
Formal Charge	0
Complexity	348
Isotope Atom Count	0
Defined Atom Stereocenter Count	10
Undefined Atom Stereocenter Count	0
Defined Bond Stereocenter Count	0
Undefined Bond Stereocenter Count	0
Covalently-Bonded Unit Count	3
Compound Is Canonicalized	Yes

► from PubChem

4 Spectral Information



4.1 1D NMR Spectra



4.1.1 1H NMR Spectra



Instrument Name	Varian CFT-20
Copyright	Copyright © 2009-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	



▶ from SpectraBase

4.1.2 ¹³C NMR Spectra



Source of Sample	Tokyo Kasei Kogyo Company, Ltd., Tokyo, Japan
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

▶ from SpectraBase

4.2 IR Spectra



4.2.1 FTIR Spectra



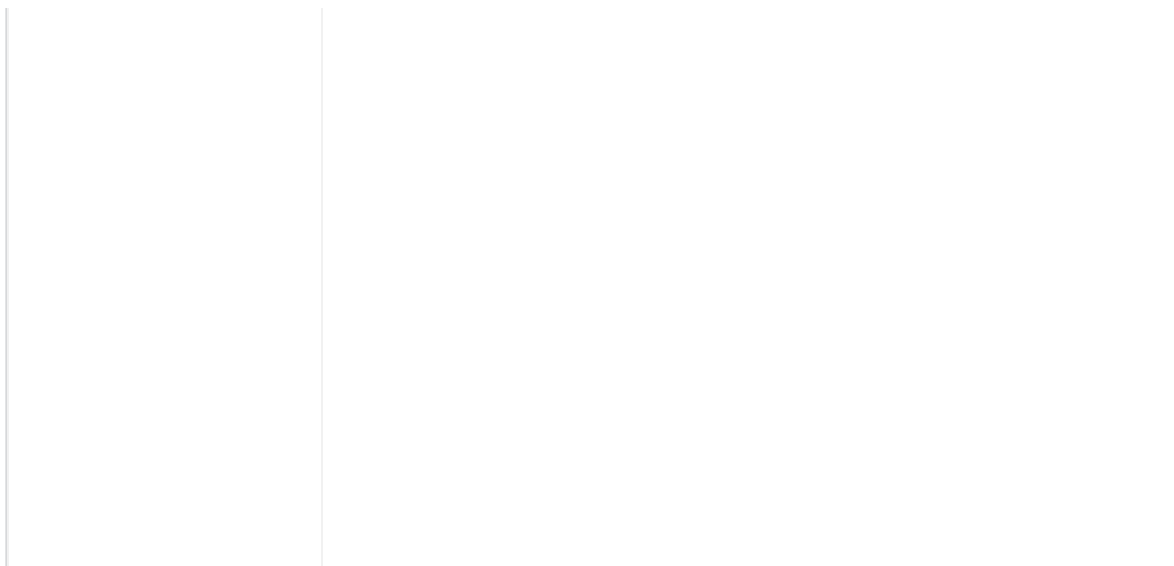
Technique	KBr WAFER
Source of Sample	Tokyo Kasei Kogyo Company, Ltd., Tokyo, Japan
Catalog Number	T 331
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

► [from SpectraBase](#)

4.2.2 ATR-IR Spectra



Instrument Name	Bio-Rad FTS
Technique	ATR-Neat (DuraSamplIR II) ground
Source of Spectrum	Forensic Spectral Research
Source of Sample	Calbiochem, EMD Chemicals, Inc., an Affiliate of Merck KGaA, Darmstadt, Germany
Catalog Number	6164
Lot Number	500894
Copyright	Copyright © 2009-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	



► from SpectraBase

Instrument Name	Bruker Tensor 27 FT-IR
Technique	ATR-Neat (DuraSAMPLIR II)
Source of Spectrum	Bio-Rad Laboratories, Inc.
Source of Sample	Spectrochem Pvt. Ltd.
Catalog Number	120282
Copyright	Copyright © 2014-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

▶ from SpectraBase

4.3 Raman Spectra



Instrument Name	Bruker MultiRAM Stand Alone FT-Raman Spectrometer
Technique	FT-Raman
Source of Spectrum	Bio-Rad Laboratories
Source of Sample	Spectrochem Pvt. Ltd., India
Catalog Number	120282
Copyright	Copyright © 2014-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

▶ from SpectraBase

5 Related Records



5.1 Related Compounds with Annotation



▶ from PubChem

5.2 Parent Compound



7427

▶ from PubChem

5.3 Related Compounds



Same Connectivity	10 Records
Same Parent, Connectivity	192 Records
Same Parent, Stereo	45 Records
Same Parent, Isotope	166 Records
Same Parent, Exact	33 Records
Mixtures, Components, and Neutralized Forms	2 Records
Similar Compounds	4,735 Records

▶ from PubChem

5.4 Substances



5.4.1 Related Substances



Same

77 Records

▶ from PubChem

5.4.2 Substances by Category



▶ from PubChem

6 Chemical Vendors



▶ from PubChem

7 Food Additives and Ingredients



7.1 FEMA Flavor Profile



At low levels can alter the perception of sweetness and alter the perception of various flavor and taste characteristics; does not impart sweetness at the levels used as a flavoring ingredient

▶ from Flavor and Extract Manufacturers Association (FEMA)

7.2 FDA Substances Added to Food



Substance	TREHALOSE, DIHYDRATE
Used for (Technical Effect)	FLAVORING AGENT OR ADJUVANT

▶ from FDA Center for Food Safety and Applied Nutrition (CFSAN)

8 Use and Manufacturing



8.1 Uses



EPA CPDat Chemical and Product Categories

▶ from EPA Chemical and Products Database (CPDat)

9 Literature



9.1 Springer Nature References



▶ from Springer Nature

9.2 Chemical Co-Occurrences in Literature



▶ from PubChem

9.3 Chemical-Disease Co-Occurrences in Literature



▶ from PubChem

9.4 Chemical-Gene Co-Occurrences in Literature



► from PubChem

10 Patents



10.1 Depositor-Supplied Patent Identifiers



▶ from PubChem

[Link to all deposited patent identifiers](#)

▶ from PubChem

11 Biological Test Results



11.1 BioAssay Results



▶ from PubChem

12 Classification



12.1 Ontologies



12.1.1 WIPO IPC



▶ from WIPO

12.1.2 ChemIDplus



▶ from ChemIDplus

12.1.3 EPA CPDat Classification



► from EPA Chemical and Products Database (CPDat)

13 Information Sources



FILTER BY SOURCE

ALL SOURCES



1. ChemIDplus

alpha, alpha-Trehalose dihydrate

<https://chem.nlm.nih.gov/chemidplus/sid/0006138234>

ChemIDplus Chemical Information Classification

<https://chem.sis.nlm.nih.gov/chemidplus/>

2. EPA DSSTox

Trehalose dihydrate

<https://comptox.epa.gov/dashboard/DTXSID3047972>

3. European Chemicals Agency (ECHA)

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

α-D-Glucopyranoside, α-D-glucopyranosyl, hydrate (1:2)

<https://echa.europa.eu/substance-information/-/substanceinfo/100.123.002>

4. EPA Chemical and Products Database (CPDat)

LICENSE

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

?-d-glucopyranoside, ?-d-glucopyranosyl, hydrate (1:2)

<https://comptox.epa.gov/dashboard/DTXSID3047972#exposure>

EPA CPDat Classification

<https://www.epa.gov/chemical-research/chemical-and-products-database-cpdatt>

5. FDA Center for Food Safety and Applied Nutrition (CFSAN)

TREHALOSE, DIHYDRATE

<https://www.accessdata.fda.gov/scripts/fdcc/?set=FoodSubstances&id=TREHALOSEDIIHYDRATE>

6. FDA/SPL Indexing Data

7YIN7J07X4

<https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/>

7. Flavor and Extract Manufacturers Association (FEMA)

TREHALOSE, DIHYDRATE

<https://www.femaflavor.org/flavor-library/trehalose-dihydrate>

8. SpectraBase

<https://spectrabase.com/spectrum/GX3tKh4xhP0>

<https://spectrabase.com/spectrum/IXLLx1oD7o8>

<https://spectrabase.com/spectrum/LHzivfDKTcx>

<https://spectrabase.com/spectrum/3wCrxhtlafr>

<https://spectrabase.com/spectrum/IW2eqfeK5BG>

<https://spectrabase.com/spectrum/5gUmQKw84kM>

9. Springer Nature

10. Wikipedia

trehalose dihydrate

<https://www.wikidata.org/wiki/Q27269028>

11. PubChem

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

12. WIPO

International Patent Classification

<http://www.wipo.int/classifications/ipc/>

