

COMPOUND SUMMARY

2-Morpholinoethanesulfonic acid hydrate

Cite

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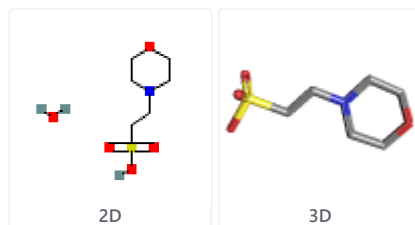
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PubChem CID: 16218417

Structure:


[Find Similar Structures](#)

Chemical Safety:



Irritant

[Laboratory Chemical Safety Summary \(LCSS\) Datasheet](#)
Molecular Formula: $C_6H_{15}NO_5S$

Chemical Names:

145224-94-8
 MES monohydrate
 2-Morpholinoethanesulfonic acid hydrate
 MES hydrate
 MFCD00149409

Molecular Weight: 213.25 g/mol

Dates:

Modify: 2019-08-10 Create: 2007-07-16

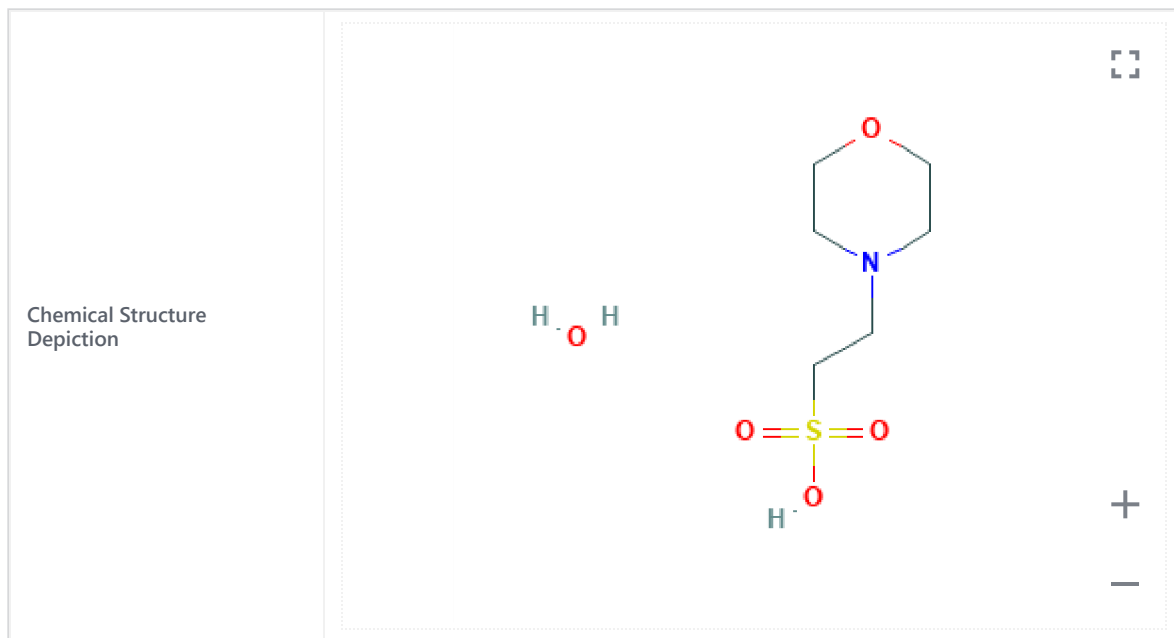
1 Structures



1.1 2D Structure



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▶ 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-morpholin-4-ylethanesulfonic acid;hydrate

▶ from PubChem

2.1.2 InChI



InChI=1S/C6H13NO4S.H2O/c8-12(9,10)6-3-7-1-4-11-5-2-7;/h1-6H2,(H,8,9,10);1H2

▶ from PubChem

2.1.3 InChI Key



MIIIXQJBDGSIKL-UHFFFAOYSA-N

▶ from PubChem

2.1.4 Canonical SMILES



C1COCCN1CCS(=O)(=O)O.O

▶ from PubChem

2.2 Molecular Formula



C₆H₁₅NO₅S

▶ from PubChem

2.3 Other Identifiers



2.3.1 CAS



145224-94-8

▶ from EPA DSSTox; European Chemicals Agency (ECHA)

2.3.2 European Community (EC) Number



919-085-9

▶ from European Chemicals Agency (ECHA)

2.4 Synonyms



2.4.1 Depositor-Supplied Synonyms



145224-94-8	MES monohydrate, 99+%, for biochemistry	DTXSID80584934
MES monohydrate	2-(N-Morpholino)ethanesulfonic acid hydrate	MIIIXQJBDGSIKL-UHF
2-Morpholinoethanesulfonic acid hydrate	4-AethssoOO>>CEa	ZX-AFC001329
MES hydrate	mes (buffer) hydrate	ANW-43959
MFCD00149409	ACMC-209umh	GB1307
4-Morpholineethanesulfonic acid monohydrate	KSC179A4H	2-(n-morpholino) eth
4-Morpholineethanesulfonic acid, monohydrate	SCHEMBL108075	AKOS000503009
2-(4-morpholinyl)ethanesulfonic acid hydrate	ARONIS014394	MES-buffered saline (
MES Hydrate Buffer	B-MES250	4-Morpholinoethanes
AK-46668	MES monohydrate, p.a., 99%	MES hydrate, >=99.5
4-Morpholineethanesulfonicacid, hydrate (1:1)	CTK0H9043	KS-000044U9
M-3055	KS-00000CMK	MES, 0.5M buffer sol
MESmonohydrate	BIB2012	DS-13905

[▶ from PubChem](#)

3 Chemical and Physical Properties



3.1 Computed Properties



Property Name	Property Value
Molecular Weight	213.25 g/mol
Hydrogen Bond Donor Count	2
Hydrogen Bond Acceptor Count	6
Rotatable Bond Count	3
Exact Mass	213.067094 g/mol
Monoisotopic Mass	213.067094 g/mol
Topological Polar Surface Area	76.2 A ²
Heavy Atom Count	13
Formal Charge	0
Complexity	214
Isotope Atom Count	0
Defined Atom Stereocenter Count	0
Undefined Atom Stereocenter Count	0
Defined Bond Stereocenter Count	0
Undefined Bond Stereocenter Count	0
Covalently-Bonded Unit Count	2
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

4.2 IR Spectra



4.2.1 FTIR Spectra



Technique	KBr WAFER
Source of Sample	Fluka Chemie AG, Buchs, Switzerland
Catalog Number	69892
Copyright	Copyright © 1980, 1981-2018 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



78165

▶ from PubChem

5.3 Related Compounds



Same Parent, Connectivity	25 Records
Same Parent, Exact	24 Records
Mixtures, Components, and Neutralized Forms	2 Records
Similar Compounds	43 Records

▶ from PubChem

5.4 Substances



5.4.1 Related Substances



Same	85 Records
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▶ from PubChem

5.4.2 Substances by Category



▶ from PubChem

6 Chemical Vendors



▶ from PubChem

7 Safety and Hazards




7.1 Hazards Identification



7.1.1 GHS Classification



Showing 1 of 2 View More

Pictogram(s)	 Irritant
Signal	Warning

GHS Hazard Statements	<p>Aggregated GHS information provided by 7 companies from 3 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.</p> <p>H315 (100%): Causes skin irritation [Warning Skin corrosion/irritation]</p> <p>H319 (100%): Causes serious eye irritation [Warning Serious eye damage/eye irritation]</p> <p>H335 (71.43%): May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation]</p> <p>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.</p>
Precautionary Statement Codes	<p>P261, P264, P271, P280, P302+P352, P304+P340, P305+P351+P338, P312, P321, P332+P313, P337+P313, P362, P403+P233, P405, and P501</p> <p>(The corresponding statement to each P-code can be found at the GHS Classification page.)</p>

▶ from European Chemicals Agency (ECHA)

8 Literature



8.1 Springer Nature References



▶ from Springer Nature

8.2 Chemical Co-Occurrences in Literature



▶ from PubChem

8.3 Chemical-Disease Co-Occurrences in Literature



▶ from PubChem

8.4 Chemical-Gene Co-Occurrences in Literature



▶ from PubChem

9 Patents



9.1 Depositor-Supplied Patent Identifiers



▶ from PubChem

10 Classification



10.1 Ontologies



10.1.1 WIPO IPC



▶ from WIPO

10.1.2 UN GHS Classification



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

11 Information Sources



FILTER BY SOURCE

ALL SOURCES



1. EPA DSSTox

2-(Morpholin-4-yl)ethane-1-sulfonic acid--water (1/1)
<https://comptox.epa.gov/dashboard/DTXSID80584934>

2. European Chemicals Agency (ECHA)

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

4-Morpholineethanesulfonic acid, hydrate (1:1)
<https://echa.europa.eu/substance-information/-/substanceinfo/100.129.173>

2-Morpholinoethanesulphonic acid
<https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/113754>

2-(morpholin-4-yl)ethane-1-sulfonic acid hydrate
<https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/163643>

3. SpectraBase

<https://spectrabase.com/spectrum/58t0UUIKGT>

<https://spectrabase.com/spectrum/AlFRGKTPG3f>

4. **Springer Nature**

5. **PubChem**

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

6. **WIPO**

International Patent Classification

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

7. **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