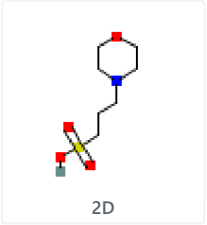
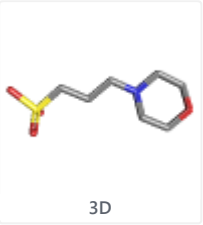
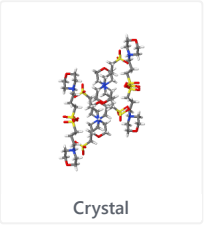
PubChem

COMPOUND SUMMARY

# 3[N-Morpholino]propane sulfonic acid

| | |
|---|---|
| PubChem CID: | 70807 |
| Structure: |  2D  3D  Crystal<br>Find Similar Structures |
| Chemical Safety: |  Irritant<br>Laboratory Chemical Safety Summary (LCSS) Datasheet |
| Molecular Formula: | $C_7H_{15}NO_4S$ |
| Chemical Names: | MOPS<br>1132-61-2<br>4-Morpholinepropanesulfonic acid<br>3-Morpholinopropanesulfonic acid<br>3-(N-Morpholino)propanesulfonic acid<br>More... |
| Molecular Weight: | 209.27 g/mol |
| Dates: | Modify: 2019-08-10 Create: 2005-03-26 |

Cite Download

CONTENTS

3-(N-morpholino)propanesulfonic acid is a Good's buffer substance, pKa = 7.2 at 20 degreeC. It is a member of morpholines, a MOPS and an organosulfonic acid. It is a conjugate acid of a 3-(N-morpholino)propanesulfonate. It is a tautomer of a 3-(N-morpholiniumyl)propanesulfonate.

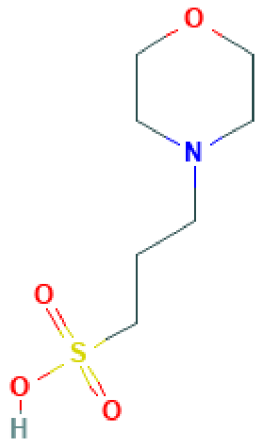
from ChEBI

# 1 Structures

## 1.1 2D Structure

Find Similar Structures | Get Image | Download

Chemical Structure Depiction




from PubChem

## 1.2 3D Conformer

from PubChem

## 1.3 Crystal Structures

| | |
|---|---|
| CCDC Number | 287618 |
| Crystal Structure Data | DOI:10.5517/cc9n907 |
| Crystal Structure Depiction | |
| Associated Article | DOI:10.1107/S1600536805027728 |

from The Cambridge Structural Database

# 2 Names and Identifiers

## 2.1 Computed Descriptors

### 2.1.1 IUPAC Name

3-morpholin-4-ylpropane-1-sulfonic acid

from PubChem

### 2.1.2 InChI

InChI=1S/C7H15NO4S/c9-13(10,11)7-1-2-8-3-5-12-6-4-8/h1-7H2,(H,9,10,11)

from PubChem

### 2.1.3 InChI Key

DVLFYONBTKHTER-UHFFFAOYSA-N

from PubChem

### 2.1.4 Canonical SMILES

C1COCCN1CCCS(=O)(=O)O

from PubChem

## 2.2 Molecular Formula

$C_7H_{15}NO_4S$

from PubChem

## 2.3 Other Identifiers

### 2.3.1 CAS

1132-61-2

- from ChemIDplus; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA)

### 2.3.2 European Community (EC) Number

214-478-5

- from European Chemicals Agency (ECHA)

### 2.3.3 UNII

273BP63NV3

- from FDA/SPL Indexing Data

### 2.3.4 Wikipedia

3-(N-morpholino)propanesulfonic acid

- from Wikipedia

## 2.4 Synonyms

### 2.4.1 MeSH Entry Terms

MOPS
morpholine propanesulphonic acid
morpholinopropane sulfonic acid

- from MeSH

### 2.4.2 Depositor-Supplied Synonyms

| | | |
|---|---|---|
| MOPS | 3-morpholin-4-ylpropane-1-sulfonic acid | 3-morpholin-4-ylpropanes |
| 1132-61-2 | 4-Morpholinopropanesulphonic acid | MPO |
| 4-Morpholinepropanesulfonic acid | 3-(morpholin-4-yl)propane-1-sulfonic acid | MOPS, 3-(N-Morpholino)p |
| 3-Morpholinopropanesulfonic acid | EINECS 214-478-5 | 2axi |
| 3-(N-Morpholino)propanesulfonic acid | BRN 1106776 | MOPS, 99.5%, for molecul |
| 3-Morpholinopropane-1-sulfonic acid | CHEBI:44115 | 3-(4-Morpholino)propane |
| Morpholinopropane sulfonic acid | DVLFYONBTKHTER-UHFFFAOYSA-N | AC1L2EWM |
| 4-Morpholinepropane sulfonic acid | 273BP63NV3 | bmse000788 |
| 3-N-Morpholinopropanesulfonic acid | 3-(4-Morpholino)propanesulfonicacid | bmse000893 |
| 3[N-MORPHOLINO]PROPANE SULFONIC ACID | 3-(4-Morpholino)propanesulfonic acid | AC1Q6X8J |
| MFCD00006183 | MOPS, Free Acid, ULTROL® Grade | DSSTox_CID_24371 |
| Morpholinopropanesulfonic acid | MOPS, 99%, for biochemistry | DSSTox_RID_80178 |
| UNII-273BP63NV3 | 3-[N-Morpholino]propanesulfonic acid | DSSTox_GSID_44371 |

from PubChem

# 3 Chemical and Physical Properties

## 3.1 Computed Properties

| Property Name | Property Value |
|---|---|
| Molecular Weight | 209.27 g/mol |
| XLogP3-AA | -3.1 |
| Hydrogen Bond Donor Count | 1 |
| Hydrogen Bond Acceptor Count | 5 |
| Rotatable Bond Count | 4 |
| Exact Mass | 209.072179 g/mol |
| Monoisotopic Mass | 209.072179 g/mol |
| Topological Polar Surface Area | 75.2 A^2 |
| Heavy Atom Count | 13 |
| Formal Charge | 0 |
| Complexity | 227 |
| Isotope Atom Count | 0 |
| Defined Atom Stereocenter Count | 0 |

| Property Name | Property Value |
|---|---|
| Undefined Atom Stereocenter Count | 0 |
| Defined Bond Stereocenter Count | 0 |
| Undefined Bond Stereocenter Count | 0 |
| Covalently-Bonded Unit Count | 1 |
| Compound Is Canonicalized | Yes |

from PubChem

## 3.2 Experimental Properties

### 3.2.1 Physical Description

DryPowder

from EPA Chemicals under the TSCA

### 3.2.2 Melting Point

284.0°C

from EPA DSSTox

# 4 Spectral Information

## 4.1 1D NMR Spectra

| | |
|---|---|
| 1D NMR Spectra | NMRShiftDB Link |

from NMRShiftDB

### 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 | Aldrich Chemical Company, Inc., Milwaukee, Wisconsin |
| Copyright | Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved. |
| Thumbnail | |

| | |
|---|---|
| | |

from SpectraBase

## 4.2 Mass Spectrometry

### 4.2.1 GC-MS

| | |
|---|---|
| NIST Number | 231736 |
| Library | Main library |
| Total Peaks | 96 |
| m/z Top Peak | 100 |
| m/z 2nd Highest | 42 |
| m/z 3rd Highest | 56 |
| Thumbnail | |

from NIST

### 4.2.2 MS-MS

| | |
|---|---|
| NIST Number | 1118792 |

| | |
|---|---|
| Instrument Type | IT/ion trap |
| Collision Energy | 0 |
| Spectrum Type | MS2 |
| Precursor Type | [M+H]+ |
| Precursor m/z | 210.0795 |
| Total Peaks | 29 |
| m/z Top Peak | 88.2 |
| m/z 2nd Highest | 123.1 |
| m/z 3rd Highest | 166.1 |
| Thumbnail | |

from NIST

## 4.3 IR Spectra

### 4.3.1 ATR-IR Spectra

| | |
|---|---|
| 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 | 41332 |
| Copyright | Copyright © 2014-2018 Bio-Rad Laboratories, Inc. All Rights Reserved. |
| Thumbnail | |

from SpectraBase

## 4.4 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 | 41332 |
| 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 Related Compounds

| | |
|---|---|
| Same Connectivity | 2 Records |
| Same Parent, Connectivity | 22 Records |
| Same Parent, Exact | 21 Records |
| Mixtures, Components, and Neutralized Forms | 44 Records |
| Similar Compounds | 55 Records |
| Similar Conformers | 1,471 Records |

from PubChem

## 5.3 Substances

### 5.3.1 Related Substances

| | |
|---|---|
| All | 472 Records |
| Same | 247 Records |
| Mixture | 225 Records |

from PubChem

### 5.3.2 Substances by Category

from PubChem

## 5.4 Entrez Crosslinks

| | |
|---|---|
| PubMed | 239 Records |
| Protein Structures | 79 Records |

from PubChem

# 6 Chemical Vendors

from PubChem

# 7 Use and Manufacturing

## 7.1 Uses

### 7.1.1 Industry Uses

Intermediates
Laboratory chemicals

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

from EPA Chemicals under the TSCA

### 7.1.2 Consumer Uses

Non-TSCA use

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

from EPA Chemicals under the TSCA

## 7.2 General Manufacturing Information

**Industry Processing Sectors**

All other basic organic chemical manufacturing
Pharmaceutical and medicine manufacturing

from EPA Chemicals under the TSCA

**EPA TSCA Commercial Activity Status**

4-Morpholinepropanesulfonic acid: ACTIVE

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

from EPA Chemicals under the TSCA

# 8 Safety and Hazards

## 8.1 Hazards Identification

### 8.1.1 GHS Classification

| Pictogram(s) | |
|---|---|

| | |
|---|---|
| |  Irritant |
| Signal | **Warning** |
| GHS Hazard Statements | Aggregated GHS information provided by 222 companies from 15 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.<br>Reported as not meeting GHS hazard criteria by 28 of 222 companies. For more detailed information, please visit ECHA C&L website<br>Of the 13 notification(s) provided by 194 of 222 companies with hazard statement code(s):<br>H315 (98.45%): Causes skin irritation [**Warning** Skin corrosion/irritation]<br>H319 (98.45%): Causes serious eye irritation [**Warning** Serious eye damage/eye irritation]<br>H335 (97.42%): May cause respiratory irritation [**Warning** Specific target organ toxicity, single exposure; Respiratory tract irritation]<br>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. |
| Precautionary Statement Codes | P261, P264, P271, P280, P302+P352, P304+P340, P305+P351+P338, P312, P321, P332+P313, P337+P313, P362, P403+P233, P405, and P501<br>(The corresponding statement to each P-code can be found at the GHS Classification page.) |

▸ from European Chemicals Agency (ECHA)

# 9 Toxicity

## 9.1 Toxicological Information

### 9.1.1 Acute Effects

from ChemIDplus

## 10 Literature

### 10.1 Depositor Provided PubMed Citations

from PubChem

### 10.2 NLM Curated PubMed Citations

from PubChem

## 10.3 Springer Nature References

from Springer Nature

## 10.4 Chemical Co-Occurrences in Literature

from PubChem

## 10.5 Chemical-Disease Co-Occurrences in Literature

from PubChem

## 10.6 Chemical-Gene Co-Occurrences in Literature

from PubChem

# 11 Patents

## 11.1 Depositor-Supplied Patent Identifiers

from PubChem

## 12 Biomolecular Interactions and Pathways

### 12.1 Protein Bound 3-D Structures

from PDB

View 79 proteins in NCBI Structure

from PubChem

### 12.2 DrugBank Interactions

Showing 1 of 3 View More

| | |
|---|---|
| Target | Alpha-xylosidase |

| | |
|---|---|
| General Function | Xyloglucan 1,6-alpha-xylosidase activity |
| Specific Function | Can catalyze the transfer of alpha-xylosyl residue from alpha-xyloside to xylose, glucose, mannose, fructose, maltose, isomaltose, nigerose, kojibiose, sucrose and trehalose. |
| Interaction References | 1. Overington JP, Al-Lazikani B, Hopkins AL: How many drug targets are there? Nat Rev Drug Discov. 2006 Dec;5(12):993-6. [PMID: 17139284]<br>2. Imming P, Sinning C, Meyer A: Drugs, their targets and the nature and number of drug targets. Nat Rev Drug Discov. 2006 Oct;5(10):821-34. [PMID: 17016423] |

▶ from DrugBank

# 13 Biological Test Results

## 13.1 BioAssay Results

▶ from PubChem

# 14 Classification

## 14.1 Ontologies

### 14.1.1 MeSH Tree

from MeSH

### 14.1.2 ChEBI Ontology

from ChEBI

### 14.1.3 WIPO IPC

from WIPO

### 14.1.4 ChemIDplus

from ChemIDplus

### 14.1.5 UN GHS Classification

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

## 15 Information Sources

FILTER BY SOURCE ALL SOURCES

1. **ChEBI**

   *3-(N-morpholino)propanesulfonic acid*
   http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:44115

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

2. **ChemIDplus**

   *MOPS*
   https://chem.nlm.nih.gov/chemidplus/sid/0001132612

   *ChemIDplus Chemical Information Classification*
   https://chem.sis.nlm.nih.gov/chemidplus/

3. ## EPA Chemicals under the TSCA

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

*4-Morpholinepropanesulfonic acid*
*https://www.epa.gov/chemicals-under-tsca*

4. ## EPA DSSTox

*4-Morpholinepropanesulfonic acid*
*https://comptox.epa.gov/dashboard/DTXSID4044371*

5. ## European Chemicals Agency (ECHA)

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

*4-morpholinopropanesulphonic acid*
*https://echa.europa.eu/substance-information/-/substanceinfo/100.013.162*

*4-morpholinopropanesulphonic acid*
*https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/37930*

6. ## DrugBank

*http://www.drugbank.ca/drugs/DB03434#targets*

7. ## FDA/SPL Indexing Data

*273BP63NV3*
*https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/*

8. ## NIST

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

9. ## NMRShiftDB

*https://pubchem.ncbi.nlm.nih.gov/substance/22390086*

10. ## PDB

*http://www.rcsb.org/ligand/MPO*

11. ## SpectraBase

*https://spectrabase.com/spectrum/KtOqNf8Y1dI*
*https://spectrabase.com/spectrum/GhAKdJ5jzhO*
*https://spectrabase.com/spectrum/EEk39zIddV7*
*https://spectrabase.com/spectrum/2H39HEpFyN8*

12. **Springer Nature**
    *https://pubchem.ncbi.nlm.nih.gov/substance/341143757*

13. **The Cambridge Structural Database**
    *https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=287618*

14. **Wikipedia**
    *3-(N-morpholino)propanesulfonic acid*
    *https://en.wikipedia.org/wiki/MOPS*

15. **PubChem**
    *https://pubchem.ncbi.nlm.nih.gov*

16. **MeSH**
    *morpholinopropane sulfonic acid*
    *https://www.ncbi.nlm.nih.gov/mesh/67008550*
    *MeSH Tree*
    *http://www.nlm.nih.gov/mesh/meshhome.html*

17. **WIPO**
    *International Patent Classification*
    *http://www.wipo.int/classifications/ipc/*

18. **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*