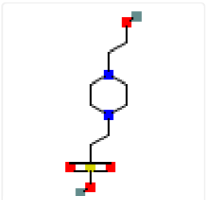
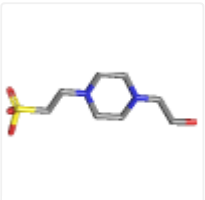
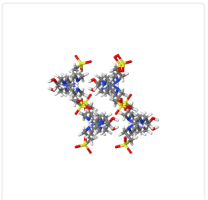
PubChem

COMPOUND SUMMARY

4-(2-Hydroxyethyl)-1-piperazine ethanesulfonic acid

PubChem CID:	23831
Structure:	 2D  3D  Crystal Find Similar Structures
Chemical Safety:	 Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula:	$C_8H_{18}N_2O_4S$
Chemical Names:	HEPES 7365-45-9 2-(4-(2-Hydroxyethyl)piperazin-1-yl)ethanesulfonic acid 4-(2-Hydroxyethyl)-1-piperazineethanesulfonic acid 1-Piperazineethanesulfonic acid, 4-(2-hydroxyethyl)- More...
Molecular Weight:	238.31 g/mol
Dates:	Modify: 2019-08-10 Create: 2004-09-16

Cite Download

CONTENTS

2-[4-(2-hydroxyethyl)piperazin-1-yl]ethanesulfonic acid is a HEPES that is **ethanesulfonic acid** in which one of the methyl hydrogens is replaced by a 4-(2-hydroxyethyl)piperazin-1-yl group. A Good's buffer substance, pKa = 7.55 at 20 degreeC. It is a HEPES and an organosulfonic acid. It is a conjugate acid of a **2-[4-(2-hydroxyethyl)piperazin-1-yl]ethanesulfonate**. It is a tautomer of a **2-[4-(2-hydroxyethyl)piperazin-4-ium-1-yl]ethanesulfonate**.

▸ from ChEBI

15(R)-hydroperoxy-EPE, also known as 4-(2-HYDROXYETHYL)-1-piperazine ethanesulfonate or Hepes, is classified as a member of the N-alkylpiperazines. N-alkylpiperazines are organic compounds containing a **piperazine** ring where the **nitrogen** ring atom carries an alkyl group. 15(R)-hydroperoxy-EPE is considered to be soluble (in **water**) and acidic

▸ from Human Metabolome Database (HMDB)

A dipolar ionic buffer.

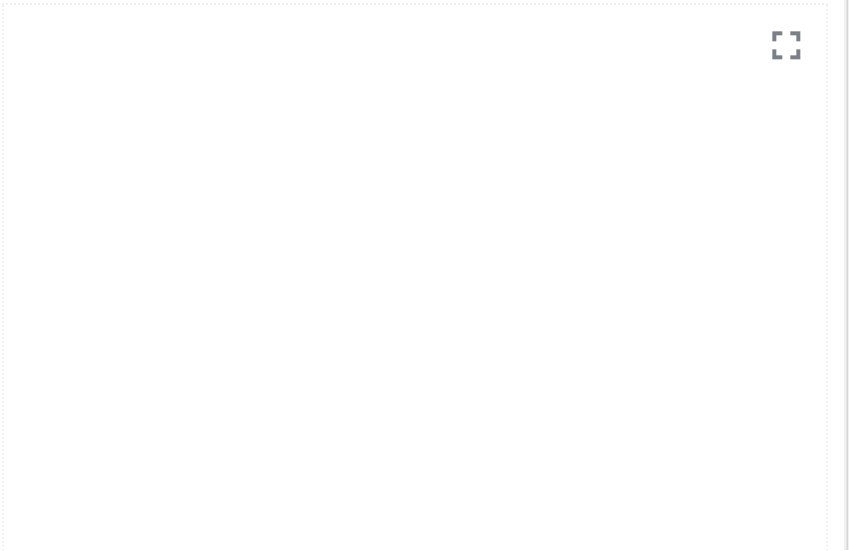
▸ from MeSH

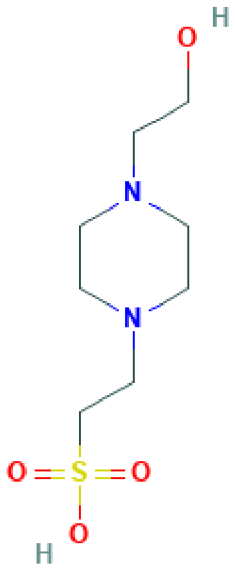
1 Structures

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

Showing 1 of 4 View More

CCDC Number	126944
Crystal Structure Data	DOI:10.5517/cc482zf
Crystal Structure Depiction	
Associated Article	DOI:10.1107/S0108270196001187

from The Cambridge Structural Database

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

2-[4-(2-hydroxyethyl)piperazin-1-yl]ethanesulfonic acid

from PubChem

2.1.2 InChI

InChI=1S/C8H18N2O4S/c11-7-5-9-1-3-10(4-2-9)6-8-15(12,13)14/h11H,1-8H2,(H,12,13,14)

from PubChem

2.1.3 InChI Key

JKMHFZQWWAIEOD-UHFFFAOYSA-N

from PubChem

2.1.4 Canonical SMILES

C1CN(CCN1CCO)CCS(=O)(=O)O

from PubChem

2.2 Molecular Formula

$C_8H_{18}N_2O_4S$

from PubChem

2.3 Other Identifiers

2.3.1 CAS

7365-45-9

from ChemIDplus; DTP/NCI; EPA Chemicals under the TSCA; European Chemicals Agency (ECHA); Human Metabolome Database (HMDB)

Related CAS

75277-39-3 (mono-hydrochloride salt)

from ChemIDplus

2.3.2 European Community (EC) Number

230-907-9

from European Chemicals Agency (ECHA)

2.3.3 NSC Number

166663

from DTP/NCI

2.3.4 UNII

RWW266YE9I

from FDA/SPL Indexing Data

2.4 Synonyms

2.4.1 MeSH Entry Terms

HEPES
HEPES Monosodium Salt
Monosodium Salt, HEPES
N 2 Hydroxyethylpiperazine N' 2' ethanesulfonic Acid
N-2-Hydroxyethylpiperazine-N'-2'-ethanesulfonic Acid
Salt, HEPES Monosodium

from MeSH

2.4.2 Depositor-Supplied Synonyms

HEPES
7365-45-9
2-(4-(2-Hydroxyethyl)piperazin-1-yl)ethanesulfonic acid
4-(2-Hydroxyethyl)-1-piperazineethanesulfonic acid
1-Piperazineethanesulfonic acid, 4-(2-hydroxyethyl)-
N-2-Hydroxyethylpiperazine-N'-ethanesulfonate
N-2-Hydroxyethylpiperazine-N'-ethanesulfonic acid
N-2-Hydroxyethylpiperazine-N-ethane sulfonic acid
NSC 166663
RWW266YE9I

2-[4-(2-hydroxyethyl)piperazin-1-yl]ethanesulfonic acid Monosodium salt, HEPES	N-2-Hydroxyethylpiperazine-N'-2'-ethanesulfonic acid JKMHFZQWWAIEOD-UHFFFAOYSA-N
4-(2-Hydroxyethyl)piperazine-1-ethanesulfonic acid	N-2-Hydroxyethylpiperazine-N'-2-ethanesulfonic acid
UNII-RWW266YE9I	N-(2-Hydroxyethyl)piperazine-N'-(2-ethanesulfonic acid)
4-(2-Hydroxyethyl)-1-piperazineethane sulfonic acid	AK-48804
MFCD00006158	EINECS 230-907-9
4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID	HEPES, 99%, for biochemistry
CHEBI:42334	2-[4-(2-Hydroxyethyl)-1-piperazinyl]ethanesulfonic acid

from PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value
Molecular Weight	238.31 g/mol
XLogP3-AA	-4
Hydrogen Bond Donor Count	2
Hydrogen Bond Acceptor Count	6
Rotatable Bond Count	5
Exact Mass	238.098728 g/mol
Monoisotopic Mass	238.098728 g/mol
Topological Polar Surface Area	89.5 A^2
Heavy Atom Count	15
Formal Charge	0
Complexity	267
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	1
Compound Is Canonicalized	Yes

from PubChem

3.2 Experimental Properties

3.2.1 Solubility

5.25e+01 g/l

ALOGPS

from Human Metabolome Database (HMDB)

3.2.2 Octanol/Water Partition Coefficient

-1.95

ALOGPS

from Human Metabolome Database (HMDB)

4 Spectral Information

4.1 1D NMR Spectra

4.1.1 1H NMR Spectra

Copyright	
Thumbnail	

from SpectraBase

4.1.2 13C NMR Spectra

Copyright	Copyright © 2006-2018 Bio-Rad Laboratories, Inc. Portions provided by BioMagResBank(BMRB) and the Board of Regents of the University of Wisconsin System. All Rights Reserved.
Thumbnail	

from SpectraBase

Source of Sample	Aldrich Chemical Company, Inc., Milwaukee, Wisconsin
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Thumbnail	

from SpectraBase

4.2 Mass Spectrometry

Showing 2 of 5 View More

MoNA ID	MoNA010747
MS Category	Experimental
MS Type	Chromatography identified as LC-MS
MS Level	MS2
Precursor Type	[M+H]+
precursor m/z	239.106018066406
Instrument	Agilent 6550 iFunnel
Instrument Type	LC-ESI-QTOF
Ionization Mode	Positive
Splash	splash10-000i-0390000000-95b81ac1152940568cab
Thumbnail	

Submitter	romanas chaleckis, gunma university

▶ from MassBank of North America (MoNA)

MoNA ID	MoNA010748
MS Category	Experimental
MS Type	Chromatography identified as LC-MS
MS Level	MS2
Precursor Type	[M+H]+
precursor m/z	239.106018066406
Instrument	Agilent 6550 iFunnel
Instrument Type	LC-ESI-QTOF
Ionization Mode	Positive
Splash	splash10-000i-0090000000-b4e4113dffb4173e7f0e
Thumbnail	

Submitter	romanas chaleckis, gunma university

▸ from MassBank of North America (MoNA)

4.2.1 GC-MS

GC-MS	GC-MS Spectrum 33914 - HMDB HMDB0062295 GC-MS Spectrum 48826 - HMDB HMDB0062295

▸ from Human Metabolome Database (HMDB)

NIST Number	230767
Library	Main library
Total Peaks	182
m/z Top Peak	112
m/z 2nd Highest	42
m/z 3rd Highest	55
Thumbnail	

from NIST

4.2.2 MS-MS

MS-MS	MS-MS Spectrum 888349 - HMDB HMDB0062295 MS-MS Spectrum 888350 - HMDB HMDB0062295 MS-MS Spectrum 888351 - HMDB HMDB0062295 MS-MS Spectrum 930094 - HMDB HMDB0062295 MS-MS Spectrum 930095 - HMDB HMDB0062295 MS-MS Spectrum 930096 - HMDB HMDB0062295

from Human Metabolome Database (HMDB)

NIST Number	1118755
Instrument Type	IT/ion trap
Collision Energy	0
Spectrum Type	MS2
Precursor Type	[M+H]+
Precursor m/z	239.106
Total Peaks	29
m/z Top Peak	131.2
m/z 2nd Highest	221.1
m/z 3rd Highest	112.2
Thumbnail	

from NIST

4.3 IR Spectra

4.3.1 FTIR Spectra

Technique	KBr WAFER
Source of Sample	Aldrich Chemical Company, Inc., Milwaukee, Wisconsin
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

from SpectraBase

4.3.2 ATR-IR Spectra

Instrument Name	Bio-Rad FTS
Technique	ATR-Neat (DuraSamplIR II)

Source of Spectrum	Forensic Spectral Research
Source of Sample	Research Organics, Inc.
Catalog Number	6003H
Lot Number	9414
Copyright	Copyright © 2009-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

from SpectraBase

4.4 Raman Spectra

Showing 2 of 3 View More

Technique	FT-Raman
Source of Spectrum	Forensic Spectral Research
Source of Sample	Research Organics, Inc.
Catalog Number	6003H
Lot Number	9414
Copyright	Copyright © 2015-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

from SpectraBase

Instrument Name	Thermo Nicolet FT-Raman 960
Technique	FT-Raman
Source of Sample	Aldrich Chemical Company, Inc.
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Thumbnail	

from SpectraBase

5 Related Records

5.1 Related Compounds with Annotation

from PubChem

5.2 Related Compounds

Same Connectivity	3 Records
Same Parent, Connectivity	79 Records
Same Parent, Exact	77 Records
Mixtures, Components, and Neutralized Forms	178 Records
Similar Compounds	102 Records
Similar Conformers	153 Records

from PubChem

5.3 Substances

5.3.1 Related Substances

All	1,426 Records
Same	1,047 Records
Mixture	379 Records

▶ from PubChem

5.3.2 Substances by Category

▶ from PubChem

5.4 Entrez Crosslinks

PubMed	13,520 Records
Protein Structures	877 Records
Taxonomy	1 Record
Gene	1 Record

from PubChem

6 Chemical Vendors

from PubChem

7 Pharmacology and Biochemistry

7.1 MeSH Pharmacological Classification

Buffers

A chemical system that functions to control the levels of specific ions in solution. When the level of hydrogen ion in solution is controlled the system is called a pH buffer. (See all compounds classified as Buffers.)

from MeSH

7.2 Human Metabolite Information

7.2.1 Metabolite Description

Description

15(R)-hydroperoxy-EPE, also known as 4-(2-HYDROXYETHYL)-1-piperazine ethanesulfonate or Hepes, is classified as a member of the N-alkylpiperazines. N-alkylpiperazines are organic compounds containing a piperazine ring where the nitrogen ring atom carries an alkyl group. 15(R)-hydroperoxy-EPE is considered to be soluble (in water) and acidic

- from Human Metabolome Database (HMDB)

8 Use and Manufacturing

8.1 Uses

8.1.1 Industry Uses

Laboratory chemicals

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

- from EPA Chemicals under the TSCA

8.2 General Manufacturing Information

Industry Processing Sectors

Wholesale and retail trade

- from EPA Chemicals under the TSCA

EPA TSCA Commercial Activity Status

1-Piperazineethanesulfonic acid, 4-(2-hydroxyethyl)-: ACTIVE

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

- from EPA Chemicals under the TSCA

9 Safety and Hazards

9.1 Hazards Identification

9.1.1 GHS Classification

Pictogram(s)	 Irritant
Signal	**Warning**
GHS Hazard Statements	Aggregated GHS information provided by 55 companies from 6 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies. Reported as not meeting GHS hazard criteria by 48 of 55 companies. For more detailed information, please visit ECHA C&L website Of the 4 notification(s) provided by 7 of 55 companies with hazard statement code(s): H302 (14.29%): Harmful if swallowed [**Warning** Acute toxicity, oral] H312 (14.29%): Harmful in contact with skin [**Warning** Acute toxicity, dermal] H315 (100%): Causes skin irritation [**Warning** Skin corrosion/irritation] H319 (100%): Causes serious eye irritation [**Warning** Serious eye damage/eye irritation] H332 (14.29%): Harmful if inhaled [**Warning** Acute toxicity, inhalation] H335 (57.14%): May cause respiratory irritation [**Warning** Specific target organ toxicity, single exposure; Respiratory tract irritation] 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, P270, P271, P280, P301+P312, P302+P352, P304+P312, P304+P340, P305+P351+P338, P312, P321, P322, P330, P332+P313, P337+P313, P362, P363, P403+P233, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)

▸ from European Chemicals Agency (ECHA)

10 Toxicity

10.1 Toxicological Information

10.1.1 Acute Effects

from ChemIDplus

11 Literature

11.1 Depositor Provided PubMed Citations

from PubChem

11.2 NLM Curated PubMed Citations

from PubChem

11.3 Springer Nature References

from Springer Nature

11.4 Thieme References

from Thieme Chemistry

11.5 Chemical Co-Occurrences in Literature

from PubChem

11.6 Chemical-Disease Co-Occurrences in Literature

from PubChem

11.7 Chemical-Gene Co-Occurrences in Literature

from PubChem

12 Patents

12.1 Depositor-Supplied Patent Identifiers

from PubChem

13 Biomolecular Interactions and Pathways

13.1 Protein Bound 3-D Structures

View 877 proteins in NCBI Structure

from PubChem

13.2 Biosystems and Pathways

from PubChem

14 Biological Test Results

14.1 BioAssay Results

from PubChem

15 Classification

15.1 Ontologies

15.1.1 MeSH Tree

from MeSH

15.1.2 ChEBI Ontology

from ChEBI

15.1.3 WIPO IPC

from WIPO

15.1.4 ChemIDplus

from ChemIDplus

15.1.5 UN GHS Classification

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

16 Information Sources

FILTER BY SOURCE ALL SOURCES

1. ## ChEBI

2-[4-(2-hydroxyethyl)piperazin-1-yl]ethanesulfonic acid
http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:42334

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

2. ## Human Metabolome Database (HMDB)

15(R)-hydroperoxy-EPE
http://www.hmdb.ca/metabolites/HMDB0062295

3. ## ChemIDplus

HEPES
https://chem.nlm.nih.gov/chemidplus/sid/0007365459

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

4. ## DTP/NCI

HEPES
https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=166663

5. ## EPA Chemicals under the TSCA

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

1-Piperazineethanesulfonic acid, 4-(2-hydroxyethyl)-
https://www.epa.gov/chemicals-under-tsca

6. ## European Chemicals Agency (ECHA)

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

4-(2-hydroxyethyl)piperazin-1-ylethanesulphonic acid
https://echa.europa.eu/substance-information/-/substanceinfo/100.028.098

4-(2-hydroxyethyl)piperazin-1-ylethanesulphonic acid
https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/119802

7. ## FDA/SPL Indexing Data

RWW266YE9I
https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/

8. ## NIST

4-(2-Hydroxyethyl)piperazine-1-ethanesulfonic acid
http://www.nist.gov/srd/nist1a.cfm

9. ## MassBank of North America (MoNA)

HEPES
http://mona.fiehnlab.ucdavis.edu/spectra/browse?inchikey=JKMHFZQWWAIEOD-UHFFFAOYSA-N

10. ## SpectraBase

https://spectrabase.com/spectrum/4gmYqOcKrZs
https://spectrabase.com/spectrum/EqENKnbFSE6
https://spectrabase.com/spectrum/Ir9uE6ISZhY
https://spectrabase.com/spectrum/1CprBXzQ7xR
https://spectrabase.com/spectrum/DTAJilgAIiL
https://spectrabase.com/spectrum/34FlQuO3BVP
https://spectrabase.com/spectrum/4zqHRGSETkA
https://spectrabase.com/spectrum/DetbaXtLOZQ

11. ## Springer Nature

12. ## The Cambridge Structural Database

https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=126944
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=248794
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=758246
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=788865

13. ## Thieme Chemistry

14. ## MeSH

HEPES
https://www.ncbi.nlm.nih.gov/mesh/68006531

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

Buffers
https://www.ncbi.nlm.nih.gov/mesh/68002021

15. ## PubChem

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

16. ## WIPO

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

17. ## 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