4-Morpholinepropanamine

Other names:	(3-Aminopropyl)morpholine 1-Amino-3-morpholinopropane 3-Morpholino-1-propylamine 3-Morpholinopropylamine 4-(3-Aminopropyl)morpholine 4-(Aminopropyl)morpholine 4-(«gamma»-Aminopropyl)morpholine 4-Morpholinepropylamine Morpholine, 4-(3-aminopropyl)- Morpholine, 4-aminopropyl- Morpholine, N-aminopropyl- N-(3-Aminopropyl)morfolin N-(3-aminopropyl)morpholine N-Aminopropylmorpholine NSC 1081 morpholine, N-(3-aminopropyl)- «gamma»-Morpholinopropylamine
Inchi:	InChI=1S/C7H16N2O/c8-2-1-3-9-4-6-10-7-5-9/h1-8H2
InchiKey:	UIKUBYKUYUSRSM-UHFFFAOYSA-N
Formula:	C7H16N2O
SMILES:	NCCCN1CCOCC1
Mol. weight [g/mol]:	144.21
CAS:	123-00-2

Physical Properties

Property code	Value	Unit	Source
log10ws	0.26		Crippen Method
logp	-0.333		Crippen Method
mcvol	124.460	ml/mol	McGowan Method
tb	497.20	K	NIST Webbook
tb	497.65	K	NIST Webbook
tf	258.15	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	296.20	J/mol×K	298.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	298.20	J/mol×K	303.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	299.60	J/mol×K	308.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	301.20	J/mol×K	313.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	302.80	J/mol×K	318.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	304.50	J/mol×K	323.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	306.10	J/mol×K	328.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	307.90	J/mol×K	333.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	309.60	J/mol×K	338.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K

cpl	311.30	J/mol×K	343.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	312.70	J/mol×K	348.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	313.40	J/mol×K	353.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
hvapt	61.80	kJ/mol	298.15	Energetic vs structural effects of aminoalkyl substituents in the morpholine

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Molar excess enthalpy (Hm E) for systems of aqueous piperazine derivatives:	https://www.doi.org/10.1016/j.jct.2015.06.006
Energetic vs structural effects of aminoalkyl substituents in the morpholine:	https://www.doi.org/10.1016/j.jct.2018.03.001
Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K:	https://www.doi.org/10.1021/je400178k
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123002&Units=SI

Legend

cpl:	Liquid phase heat capacity
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point