1,2-Ethanediamine, N-methyl-

Other names: 2-(Methylamino)ethylamine

2-Aminoethylmethylamine Ethylenediamine, N-methyl-N-Methyldiaminoethane N-Methylethanediamine N-Methylethylenediamine

Inchi: InChi=1S/C3H10N2/c1-5-3-2-4/h5H,2-4H2,1H3

InchiKey: KFIGICHILYTCJF-UHFFFAOYSA-N

 Formula:
 C3H10N2

 SMILES:
 CNCCN

 Mol. weight [g/mol]:
 74.12

 CAS:
 109-81-9

Physical Properties

Property code	Value	Unit	Source
gf	130.22	kJ/mol	Joback Method
hf	-17.99	kJ/mol	Joback Method
hfus	13.82	kJ/mol	Joback Method
hvap	39.35	kJ/mol	Joback Method
log10ws	0.30		Crippen Method
logp	-0.835		Crippen Method
mcvol	73.090	ml/mol	McGowan Method
рс	4849.43	kPa	Joback Method
tb	388.20	K	NIST Webbook
tc	579.02	K	Joback Method
tf	259.49	K	Joback Method
VC	0.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.99	J/mol×K	579.02	Joback Method
cpg	177.40	J/mol×K	547.64	Joback Method
cpg	170.50	J/mol×K	516.26	Joback Method

cpg	163.29	J/mol×K	484.88	Joback Method
cpg	155.75	J/mol×K	453.50	Joback Method
cpg	147.88	J/mol×K	422.12	Joback Method
cpg	139.67	J/mol×K	390.74	Joback Method
pvap	0.94	kPa	289.30	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
рvар	0.59	kPa	282.30	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	0.61	kPa	283.10	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	0.66	kPa	284.10	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	0.70	kPa	284.90	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	0.77	kPa	286.30	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	0.86	kPa	287.80	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	0.54	kPa	281.30	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study

pvap	1.03	kPa	290.60	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study	
pvap	1.18	kPa	292.20	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study	
pvap	1.39	kPa	294.60	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study	
pvap	1.54	kPa	296.20	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study	
pvap	1.76	kPa	298.10	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study	
pvap	2.02	kPa	300.20	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study	
pvap	2.28	kPa	302.20	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study	_
pvap	0.49	kPa	280.20	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study	_
pvap	0.47	kPa	279.40	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study	

pvap	0.45	kPa	278.60	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	0.41	kPa	278.00	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	0.34	kPa	275.40	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	0.32	kPa	274.30	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	0.27	kPa	272.20	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C109819&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Thermodynamic Properties of https://www.doi.org/10.1021/acs.jced.5b01003

N-Methyl-Substituted https://en.wikipedia.org/wiki/Joback_method

Computational Study:

Legend

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditionshfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws:Log10 of Water solubility in mol/llogp:Octanol/Water partition coefficientmcvol:McGowan's characteristic volume

pc: Critical Pressurepvap: Vapor pressure

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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