

Sym-Dimethylethylene diamine

Other names:	1,2-Bis(methylamino)ethane 1,2-Ethanediamine, N1,N2-dimethyl- 2,5-Diazahehexane CH3NHCH2CH2NHCH3 Ethylenediamine, N,N'-dimethyl- N,N'-Dimethyl-1,2-ethanediamine N,N'-Dimethyldiaminoethane N,N'-Dimethylethanediamine N,N'-Dimethylethano-1,2-diamine N,N'-Dimethylethylenediamine N1,N2-dimethylethane-1,2-diamine sym-Dimethylethylenediamine
Inchi:	InChI=1S/C4H12N2/c1-5-3-4-6-2/h5-6H,3-4H2,1-2H3
InchiKey:	KVKFRMCSXWQSNT-UHFFFAOYSA-N
Formula:	C4H12N2
SMILES:	CNCCNC
Mol. weight [g/mol]:	88.15
CAS:	110-70-3

Physical Properties

Property code	Value	Unit	Source
affp	989.20	kJ/mol	NIST Webbook
basg	946.90	kJ/mol	NIST Webbook
hf	-23.10	kJ/mol	Cheméo Relay (1.0)
hfus	16.31	kJ/mol	Joback Method
hvap	46.98	kJ/mol	Cheméo Relay (1.0)
ie	8.54	eV	Cheméo Relay (1.0)
logp	-0.575		Crippen Method
mcvol	87.180	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
tb	393.20	K	NIST Webbook
tc	569.76	K	Cheméo Relay (1.0)
tf	241.74	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.53	J/mol×K	391.26	Joback Method
cpg	218.02	J/mol×K	567.87	Joback Method
cpg	210.16	J/mol×K	538.43	Joback Method
cpg	201.95	J/mol×K	509.00	Joback Method
cpg	193.40	J/mol×K	479.56	Joback Method
cpg	184.48	J/mol×K	450.13	Joback Method
cpg	175.20	J/mol×K	420.69	Joback Method
pvap	3.97	kPa	310.70	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	0.43	kPa	279.20	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	0.86	kPa	288.20	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	1.23	kPa	293.20	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	1.50	kPa	295.80	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	1.78	kPa	298.20	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study

pvap	2.48	kPa	303.40	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	0.59	kPa	283.30	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	3.41	kPa	308.20	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	0.50	kPa	281.40	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	2.89	kPa	305.60	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	2.11	kPa	300.70	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	1.02	kPa	290.60	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study
pvap	0.69	kPa	285.60	Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56411e+01
Coeff. B	-3.77810e+03
Coeff. C	-5.04460e+01
Temperature range (K), min.	274.78
Temperature range (K), max.	416.20

Sources

Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-Diamines: Experimental and Computational Study: McGowan Method:	https://www.doi.org/10.1021/acs.jced.5b01003
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Computational Study:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110703&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0, beta):	

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure

tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

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