Cyclohexanamine, N,N-dimethyl-

Other names:	(Dimethylamino)cyclohexane
	Cyclohexylamine, N,N-dimethyl-
	Cyclohexyldimethylamine
	Dimethylcyclohexylamine
	N,N-Dimethyl-N-cyclohexylamine
	N,N-Dimethylaminocyclohexane
	N,N-Dimethylcyclohexanamine
	N,N-Dimethylcyclohexylamine
	N-Cyclohexyldimethylamine
	NSC 163904
	Polycat 8
	UN 2264
Inchi:	InChI=1S/C8H17N/c1-9(2)8-6-4-3-5-7-8/h8H,3-7H2,1-2H3
InchiKey:	SVYKKECYCPFKGB-UHFFFAOYSA-N
Formula:	C8H17N
SMILES:	CN(C)C1CCCCC1
Mol. weight [g/mol]:	127.23
CAS:	98-94-2

Physical Properties

Property code	Value	Unit	Source
affp	983.60	kJ/mol	NIST Webbook
basg	952.60	kJ/mol	NIST Webbook
chl	-5442.80 ± 2.00	kJ/mol	NIST Webbook
gf	151.71	kJ/mol	Joback Method
hf	-86.60	kJ/mol	Joback Method
hfl	-134.80 ± 2.00	kJ/mol	NIST Webbook
hfus	11.33	kJ/mol	Joback Method
hvap	35.87	kJ/mol	Joback Method
ie	7.50	eV	NIST Webbook
ie	8.09	eV	NIST Webbook
log10ws	-1.75		Crippen Method
logp	1.881		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook

rinpol	994.00		NIST Webbook
tb	431.70	K	NIST Webbook
tc	613.03	K	Joback Method
tf	219.77	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.24	J/mol×K	414.43	Joback Method
cpg	261.82	J/mol×K	447.53	Joback Method
cpg	279.47	J/mol×K	480.63	Joback Method
cpg	296.20	J/mol×K	513.73	Joback Method
cpg	312.04	J/mol×K	546.83	Joback Method
cpg	327.04	J/mol×K	579.93	Joback Method
cpg	341.20	J/mol×K	613.03	Joback Method
pvap	0.91	kPa	311.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.09	kPa	275.30	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.09	kPa	275.40	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.11	kPa	278.30	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.15	kPa	281.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.18	kPa	284.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.21	kPa	287.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study

pvap	0.09	kPa	275.30	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.32	kPa	293.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.38	kPa	296.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.47	kPa	299.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.57	kPa	302.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.66	kPa	305.30	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.81	kPa	308.30	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.26	kPa	290.30	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	1.11	kPa	314.30	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
rhol	856.40	kg/m3	283.15	Physicochemical properties of switchable-hydrophilicity solvent systems: N,N-Dimethylcyclohexylamine, water and carbon dioxide
rhol	854.00	kg/m3	288.15	Physicochemical properties of switchable-hydrophilicity solvent systems: N,N-Dimethylcyclohexylamine, water and carbon dioxide

rhol	851.50	kg/m3	293.15	Physicochemical properties of switchable-hydrophilicity solvent systems: N,N-Dimethylcyclohexylamine, water and carbon dioxide
rhol	849.10	kg/m3	298.15	Physicochemical properties of switchable-hydrophilicity solvent systems: N,N-Dimethylcyclohexylamine, water and carbon dioxide
rhol	846.50	kg/m3	303.15	Physicochemical properties of switchable-hydrophilicity solvent systems: N,N-Dimethylcyclohexylamine, water and carbon dioxide
rhol	844.00	kg/m3	308.15	Physicochemical properties of switchable-hydrophilicity solvent systems: N,N-Dimethylcyclohexylamine, water and carbon dioxide

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47617e+01
Coeff. B	-3.74877e+03
Coeff. C	-6.21220e+01
Temperature range (K), min.	321.12
Temperature range (K), max.	458.81

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermodynamic properties of cyclohexanamines: Experimental and theoretical study:	https://www.doi.org/10.1016/j.tca.2015.03.016
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Physicochemical properties of switchable-hydrophilicity solvent systems: N,N-Dimethylcyclohexylamine, water and carbon dioxide:	https://www.doi.org/10.1016/j.jct.2019.01.030

Non-random two-liquid modelling of switchable-hydrophilicity solvent systems:	https://www.doi.org/10.1016/j.fluid.2015.09.032
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98942&Units=SI
N,N-Dimethylcyclohexanamine, water, and toluene:	
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume