

1,6-Hexanediamine, N,N'-dimethyl-

Other names:	N,N'-Dimethyl-1,6-diaminohexane N,N'-Dimethyl-1,6-hexanediamine N,N'-Dimethylhexamethylenediamine N,N'-dimethylhexane-1,6-diamine
Inchi:	InChI=1S/C8H20N2/c1-9-7-5-3-4-6-8-10-2/h9-10H,3-8H2,1-2H3
InchiKey:	MDKQJOKKKZQNQDG-UHFFFAOYSA-N
Formula:	C8H20N2
SMILES:	CNCCCCCNC
Mol. weight [g/mol]:	144.26
CAS:	13093-04-4

Physical Properties

Property code	Value	Unit	Source
gf	195.26	kJ/mol	Joback Method
hf	-101.51	kJ/mol	Joback Method
hfus	26.67	kJ/mol	Joback Method
hvap	46.27	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	0.986		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
tb	482.78	K	Joback Method
tc	654.76	K	Joback Method
tf	285.24	K	Joback Method
vc	0.553	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.81	J/molxK	482.78	Joback Method
cpg	342.81	J/molxK	511.44	Joback Method
cpg	356.24	J/molxK	540.11	Joback Method
cpg	369.11	J/molxK	568.77	Joback Method
cpg	381.45	J/molxK	597.43	Joback Method

cpg	393.25	J/mol×K	626.10	Joback Method
cpg	404.54	J/mol×K	654.76	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.20	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.18171e+01
Coeff. B	-3.06135e+03
Coeff. C	-6.08030e+01
Temperature range (K), min.	326.33
Temperature range (K), max.	531.37

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13093044&Units=SI
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/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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