N-Cyclohexyl-1,3-propanediamine

Other names:	N-(3-Aminopropyl)cyclohexylamine N-Cyclohexyl-1,3-propylenediamine 3-Cyclohexylamino-1-propylamine N-Cyclohexyl trimethylene diamine N-Cyclohexyl-1,3-diaminopropane 1,3-Propanediamine, N-cyclohexyl- Cyclohexyl-1,3-propanediamine Cyclohexylamine, N-(3-aminopropyl)- N-Cyclohexylpropylene-1,3-diamine 1-(Cyclohexylamino)-3-aminopropane 3-(Aminopropyl)cyclohexylamine 1,3-Propanediamine, N1-cyclohexyl- NSC 87572 3-cyclohexylaminopropylamine
Inchi:	InChI=1S/C9H20N2/c10-7-4-8-11-9-5-2-1-3-6-9/h9,11H,1-8,10H2
InchiKey:	ITZPOSYADVYECJ-UHFFFAOYSA-N
Formula:	C9H20N2
SMILES:	NCCCNC1CCCCC1
Mol. weight [g/mol]:	156.27
CAS:	3312-60-5

Physical Properties

Property code	Value	Unit	Source
gf	205.19	kJ/mol	Joback Method
hf	-87.51	kJ/mol	Joback Method
hfus	21.20	kJ/mol	Joback Method
hvap	53.13	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	1.258		Crippen Method
mcvol	146.770	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
tb	547.57	K	Joback Method
tc	759.64	K	Joback Method
tf	334.49	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.43	J/mol×K	547.57	Joback Method
cpg	394.76	J/mol×K	582.91	Joback Method
cpg	412.05	J/mol×K	618.26	Joback Method
cpg	428.33	J/mol×K	653.60	Joback Method
cpg	443.64	J/mol×K	688.95	Joback Method
cpg	458.01	J/mol×K	724.29	Joback Method
cpg	471.47	J/mol×K	759.64	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	394.70	K	2.70	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3312605&Units=SI

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume