N-CYCLOHEXYL-1,3-PROPANEDIAMINE

Other names: 1,3-Propanediamine, N-cyclohexyl-
1,3-Propanediamine, N1-cyclohexyl-
1-(Cyclohexylamino)-3-aminopropane
3-(Aminopropyl)cyclohexylamine
3-Cyclohexylamino-1-propylamine
3-cyclohexylaminopropylamine
Cyclohexyl-1,3-propanediamine
Cyclohexylamine, N-(3-aminopropyl)-
N-(3-Aminopropyl)cyclohexylamine
N-Cyclohexyl trimethylene diamine
N-Cyclohexyl-1,3-diaminopropane
N-Cyclohexyl-1,3-propylenediamine
N-Cyclohexylpropylene-1,3-diamine
NSC 87572

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

Physical Properties

Property code	Value	Unit	Source
hfus	21.20	kJ/mol	Joback Method
logp	1.258		Crippen Method
mcvol	146.770	ml/mol	McGowan Method
tb	516.88	K	Cheméo Relay (1.0)
tf	279.16	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3312605&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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

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

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point