

N-Cyclohexylformamide

Other names:	Cyclohexylformamide Formamidocyclohexane N-Cyclohexylformamide
Inchi:	InChI=1S/C7H13NO/c9-6-8-7-4-2-1-3-5-7/h6-7H,1-5H2,(H,8,9)
InchiKey:	SWGXMLRCJNEEGZ-UHFFFAOYSA-N
Formula:	C7H13NO
SMILES:	O=CNC1CCCCC1
Mol. weight [g/mol]:	127.19

Physical Properties

Property code	Value	Unit	Source
hfus	13.11	kJ/mol	Joback Method
ie	9.22	eV	Cheméo Relay (1.0)
logp	1.065		Crippen Method
mcvol	110.180	ml/mol	McGowan Method
rinpol	1306.00		NIST Webbook
tb	502.09	K	Cheméo Relay (1.0)
tf	312.40 ± 0.60	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.63	J/mol×K	477.94	Joback Method
cpg	258.95	J/mol×K	513.35	Joback Method
cpg	273.41	J/mol×K	548.76	Joback Method
cpg	287.04	J/mol×K	584.17	Joback Method
cpg	299.87	J/mol×K	619.58	Joback Method
cpg	311.91	J/mol×K	654.99	Joback Method
cpg	323.20	J/mol×K	690.40	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	386.20	K	93.30	NIST Webbook
tbrp	418.50 ± 0.50	K	2.00	NIST Webbook

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C766938&Units=SI

Legend

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

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