Cyclohexanecarboxamide

Other names:	Cyclohexamethylene carbamide
	Cyclohexaneformamide
	Cyclohexylcarboxamide
	Cyclohexylcarboxyamide
	Hexahydrobenzoic acid amide
	Cyclohexanecarboxylic acid amide
	Hexahydrobenzamide
	NSC 16584
Inchi:	InChI=1S/C7H13NO/c8-7(9)6-4-2-1-3-5-6/h6H,1-5H2,(H2,8,9)
InchiKey:	PNZXMIKHJXIPEK-UHFFFAOYSA-N
Formula:	C7H13NO
SMILES:	NC(=O)C1CCCCC1
Mol. weight [g/mol]:	127.18
CAS:	1122-56-1

Physical Properties

Property code	Value	Unit	Source
gf	-29.96	kJ/mol	Joback Method
hf	-212.28	kJ/mol	Joback Method
hfus	12.52	kJ/mol	Joback Method
hvap	48.99	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.052		Crippen Method
mcvol	110.180	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
tb	505.51	K	Joback Method
tc	734.07	K	Joback Method
tf	309.22	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.28	J/mol×K	505.51	Joback Method

cpg	269.84	J/mol×K	543.60	Joback Method
cpg	284.46	J/mol×K	581.70	Joback Method
cpg	298.15	J/mol×K	619.79	Joback Method
cpg	310.95	J/mol×K	657.88	Joback Method
cpg	322.89	J/mol×K	695.97	Joback Method
cpg	333.99	J/mol×K	734.07	Joback Method

Sources

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=C1122561&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume