Cyclohexanone, 2-[(dimethylamino)methyl]-

Other names: 2-(N,N-Dimethylaminomethyl)cyclohexanone
2-[(Dimethylamino)methyl]cyclohexanone
2-[(dimethylamino)methyl]cyclohexan-1-one
Inchi: InChI=1S/C9H17NO/c1-10(2)7-8-5-3-4-6-9(8)11/h8H,3-7H2,1-2H3
InchiKey: QDHLEFBSGUGHCL-UHFFFAOYSA-N
Formula: C9H17NO
SMILES: CN(C)CC1CCCCC1=O
Mol. weight [g/mol]: 155.24
CAS: 15409-60-6

Physical Properties

Property code	Value	Unit	Source
gf	37.54	kJ/mol	Joback Method
hf	-244.94	kJ/mol	Joback Method
hfus	13.43	kJ/mol	Joback Method
hvap	42.35	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	1.307		Crippen Method
mcvol	138.360	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	505.13	K	Joback Method
tc	718.91	K	Joback Method
tf	299.26	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.78	J/mol×K	505.13	Joback Method
cpg	344.54	J/mol×K	540.76	Joback Method
cpg	362.37	J/mol×K	576.39	Joback Method
cpg	379.28	J/mol×K	612.02	Joback Method
cpg	395.27	J/mol×K	647.65	Joback Method
cpg	410.36	J/mol×K	683.28	Joback Method

cpg	424.55	J/mol×K	718.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15409606&Units=SI
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

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