N-Acetyl-N-methylcyclohexanamine

Other names: Cyclohexanamine, N-acetyl, N-methyl-
Inchi: InChI=1S/C9H17NO/c1-8(11)10(2)9-6-4-3-5-7-9/h9H,3-7H2,1-2H3
InchiKey: NVEYVSRXOFPIRE-UHFFFAOYSA-N
Formula: C9H17NO
SMILES: CC(=O)N(C)C1CCCCC1
Mol. weight [g/mol]: 155.24

Physical Properties

Property code	Value	Unit	Source
gf	31.21	kJ/mol	Joback Method
hf	-219.82	kJ/mol	Joback Method
hfus	15.52	kJ/mol	Joback Method
hvap	44.85	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.797		Crippen Method
mcvol	138.360	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
rinpol	1441.00		NIST Webbook
rinpol	1441.00		NIST Webbook
tb	491.18	K	Joback Method
tc	698.59	K	Joback Method
tf	280.97	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.98	J/mol×K	491.18	Joback Method
cpg	334.27	J/mol×K	525.75	Joback Method
cpg	351.54	J/mol×K	560.32	Joback Method
cpg	367.81	J/mol×K	594.88	Joback Method
cpg	383.12	J/mol×K	629.45	Joback Method
cpg	397.51	J/mol×K	664.02	Joback Method
cpg	411.00	J/mol×K	698.59	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=U373182&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume