1-N-methylaminoadamantane

Other names: 1-Methylaminoadamantane
Inchi: InChI=1S/C11H19N/c1-12-11-5-8-2-9(6-11)4-10(3-8)7-11/h8-10,12H,2-7H2,1H3/t8-,9+,1
InchiKey: NZOLSRPWNVZXTK-BIBSGERRSA-N
Formula: C11H19N
SMILES: CNC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 165.28
CAS: 3717-38-2

Physical Properties

Property code	Value	Unit	Source
gf	288.08	kJ/mol	Joback Method
hf	-9.76	kJ/mol	Joback Method
hfus	16.42	kJ/mol	Joback Method
hvap	44.97	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.175		Crippen Method
mcvol	143.250	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
rinpol	1345.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1387.00		NIST Webbook
tb	521.31	K	Joback Method
tc	742.08	K	Joback Method
tf	336.35	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.28	J/mol×K	521.31	Joback Method
cpg	397.14	J/mol×K	558.11	Joback Method
cpg	416.37	J/mol×K	594.90	Joback Method

cpg	434.20	J/mol×K	631.70	Joback Method
cpg	450.81	J/mol×K	668.49	Joback Method
cpg	466.40	J/mol×K	705.29	Joback Method
cpg	481.18	J/mol×K	742.08	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=C3717382&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