2-N-methylaminoadamantane

Other names: 2-Methylaminoadamantane
Inchi: InChI=1S/C11H19N/c1-12-11-9-3-7-2-8(5-9)6-10(11)4-7/h7-12H,2-6H2,1H3
InchiKey: VSKMVAJFNWCWPG-UHFFFAOYSA-N
Formula: C11H19N
SMILES: CNC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 165.28

Physical Properties

Property code	Value	Unit	Source
gf	285.86	kJ/mol	Joback Method
hf	-45.34	kJ/mol	Joback Method
hfus	23.79	kJ/mol	Joback Method
hvap	45.81	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.030		Crippen Method
mcvol	143.250	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	1390.00		NIST Webbook
rinpol	1390.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1390.00		NIST Webbook
tb	516.40	K	Joback Method
tc	728.05	K	Joback Method
tf	308.21	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.76	J/mol×K	516.40	Joback Method
cpg	398.08	J/mol×K	551.68	Joback Method
cpg	418.00	J/mol×K	586.95	Joback Method
cpg	436.62	J/mol×K	622.23	Joback Method
cpg	454.02	J/mol×K	657.50	Joback Method

cpg	470.30	J/mol×K	692.78	Joback Method
cpg	485.54	J/mol×K	728.05	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=R44352&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

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