2-Adamantylamine, N-acetyl-

Inchi: InChI=1S/C12H19NO/c1-7(14)13-12-10-3-8-2-9(5-10)6-11(12)4-8/h8-12H,2-6H2,1H3,(H,
InchiKey: OFEZUSBZKMXQEU-UHFFFAOYSA-N
Formula: C12H19NO
SMILES: CC(=O)NC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 193.29
CAS: 52917-72-3

Physical Properties

Property code	Value	Unit	Source
gf	165.36	kJ/mol	Joback Method
hf	-178.56	kJ/mol	Joback Method
hfus	27.98	kJ/mol	Joback Method
hvap	54.78	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	1.947		Crippen Method
mcvol	158.910	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
rinpol	1761.00		NIST Webbook
tb	593.15	K	Joback Method
tc	809.47	K	Joback Method
tf	369.41	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.59	J/mol×K	593.15	Joback Method
cpg	475.34	J/mol×K	629.20	Joback Method
cpg	493.76	J/mol×K	665.26	Joback Method
cpg	510.94	J/mol×K	701.31	Joback Method
cpg	526.99	J/mol×K	737.36	Joback Method
cpg	541.99	J/mol×K	773.42	Joback Method
cpg	556.06	J/mol×K	809.47	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52917723&Units=SI

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