Acetyldamantane

Inchi: InChI=1S/C12H18O/c1-8(13)12-5-9-2-10(6-12)4-11(3-9)7-12/h9-11H,2-7H2,1H3/t9-,10+,
InchiKey: DACIGVIOAFXPHW-CDECOKDKSA-N
Formula: C12H18O
SMILES: CC(=O)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
gf	78.19	kJ/mol	Joback Method
hf	-196.45	kJ/mol	Joback Method
hfus	15.51	kJ/mol	Joback Method
hvap	47.50	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.792		Crippen Method
mcvol	148.930	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	1888.00		NIST Webbook
rinpol	1888.00		NIST Webbook
tb	547.89	K	Joback Method
tc	773.67	K	Joback Method
tf	344.89	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.75	J/mol×K	547.89	Joback Method
cpg	416.77	J/mol×K	585.52	Joback Method
cpg	435.26	J/mol×K	623.15	Joback Method
cpg	452.43	J/mol×K	660.78	Joback Method
cpg	468.48	J/mol×K	698.41	Joback Method
cpg	483.63	J/mol×K	736.04	Joback Method
cpg	498.09	J/mol×K	773.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418665&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume