1-Adamantanol, acetate

Inchi: InChI=1S/C12H18O2/c1-8(13)14-12-5-9-2-10(6-12)4-11(3-9)7-12/h9-11H,2-7H2,1H3
InchiKey: ZYLRDAOEBRPIGT-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: CC(=O)OC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	-26.81	kJ/mol	Joback Method
hf	-328.67	kJ/mol	Joback Method
hfus	16.70	kJ/mol	Joback Method
hvap	49.91	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.518		Crippen Method
mcvol	154.800	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1458.00		NIST Webbook
rinpol	1458.00		NIST Webbook
tb	570.31	K	Joback Method
tc	793.24	K	Joback Method
tf	367.12	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.27	J/mol×K	570.31	Joback Method
cpg	443.51	J/mol×K	607.47	Joback Method
cpg	461.41	J/mol×K	644.62	Joback Method
cpg	478.15	J/mol×K	681.78	Joback Method
cpg	493.91	J/mol×K	718.93	Joback Method
cpg	508.89	J/mol×K	756.09	Joback Method
cpg	523.27	J/mol×K	793.24	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=R44320&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