Adamantan-1-ol, 2,2-dimethyl

Inchi: InChI=1S/C12H20O/c1-11(2)10-4-8-3-9(5-10)7-12(11,13)6-8/h8-10,13H,3-7H2,1-2H3
InchiKey: UPEAISCZLTUNGL-UHFFFAOYSA-N
Formula: C12H20O
SMILES: CC1(C)C2CC3CC(C2)CC1(O)C3
Mol. weight [g/mol]: 180.29

Physical Properties

Property code	Value	Unit	Source
gf	57.09	kJ/mol	Joback Method
hf	-241.20	kJ/mol	Joback Method
hfus	12.78	kJ/mol	Joback Method
hvap	55.98	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.584		Crippen Method
mcvol	153.230	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
rinpol	1253.00		NIST Webbook
tb	581.77	K	Joback Method
tc	791.02	K	Joback Method
tf	375.44	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.92	J/mol×K	581.77	Joback Method
cpg	455.50	J/mol×K	616.65	Joback Method
cpg	471.94	J/mol×K	651.52	Joback Method
cpg	487.46	J/mol×K	686.40	Joback Method
cpg	502.32	J/mol×K	721.27	Joback Method
cpg	516.76	J/mol×K	756.15	Joback Method
cpg	531.01	J/mol×K	791.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R13026&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

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