3,5-dimethyl-1-hydroxymethyladamantane

Inchi: InChI=1S/C13H22O/c1-11-3-10-4-12(2,6-11)8-13(5-10,7-11)9-14/h10,14H,3-9H2,1-2H3
InchiKey: RVWLWJAOIBEWAV-UHFFFAOYSA-N
Formula: C13H22O
SMILES: CC12CC3CC(C)(C1)CC(CO)(C3)C2
Mol. weight [g/mol]: 194.31

Physical Properties

Property code	Value	Unit	Source
gf	67.73	kJ/mol	Joback Method
hf	-226.26	kJ/mol	Joback Method
hfus	8.00	kJ/mol	Joback Method
hvap	57.36	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.975		Crippen Method
mcvol	167.320	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
rinpol	1425.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1425.00		NIST Webbook
ripol	2017.00		NIST Webbook
ripol	2032.00		NIST Webbook
ripol	2017.00		NIST Webbook
tb	609.56	K	Joback Method
tc	823.34	K	Joback Method
tf	414.85	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.07	J/mol×K	609.56	Joback Method
cpg	502.30	J/mol×K	645.19	Joback Method

cpg	518.57	J/mol×K	680.82	Joback Method
cpg	534.23	J/mol×K	716.45	Joback Method
cpg	549.63	J/mol×K	752.08	Joback Method
cpg	565.11	J/mol×K	787.71	Joback Method
cpg	581.02	J/mol×K	823.34	Joback Method

Sources

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=R304675&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume