2-methyl-1-hydroxymethyladamantane

Inchi: InChI=1S/C12H20O/c1-8-11-3-9-2-10(4-11)6-12(8,5-9)7-13/h8-11,13H,2-7H2,1H3
InchiKey: QIYMDQBSEMTZPK-UHFFFAOYSA-N
Formula: C12H20O
SMILES: CC1C2CC3CC(C2)CC1(CO)C3
Mol. weight [g/mol]: 180.29

Physical Properties

Property code	Value	Unit	Source
gf	62.58	kJ/mol	Joback Method
hf	-256.44	kJ/mol	Joback Method
hfus	19.07	kJ/mol	Joback Method
hvap	57.13	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.441		Crippen Method
mcvol	153.230	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
rinpol	1490.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1504.00		NIST Webbook
ripol	2167.00		NIST Webbook
ripol	2167.00		NIST Webbook
tb	581.53	K	Joback Method
tc	783.10	K	Joback Method
tf	351.54	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.53	J/mol×K	581.53	Joback Method
cpg	457.35	J/mol×K	615.12	Joback Method
cpg	474.05	J/mol×K	648.72	Joback Method

cpg	489.79	J/mol×K	682.31	Joback Method
cpg	504.70	J/mol×K	715.91	Joback Method
cpg	518.95	J/mol×K	749.50	Joback Method
cpg	532.67	J/mol×K	783.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R304591&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume