1-hydroxymethyladamantane

Inchi: InChI=1S/C11H18O/c12-7-11-4-8-1-9(5-11)3-10(2-8)6-11/h8-10,12H,1-7H2
InchiKey: MDVGOOIANLZFCP-UHFFFAOYSA-N
Formula: C11H18O
SMILES: OCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 166.26

Physical Properties

Property code	Value	Unit	Source
gf	61.87	kJ/mol	Joback Method
hf	-215.46	kJ/mol	Joback Method
hfus	15.41	kJ/mol	Joback Method
hvap	55.21	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.195		Crippen Method
mcvol	139.140	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpol	1423.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1455.00		NIST Webbook
ripol	2053.00		NIST Webbook
ripol	2053.00		NIST Webbook
ripol	2072.00		NIST Webbook
tb	563.32	K	Joback Method
tc	768.03	K	Joback Method
tf	344.51	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.32	J/mol×K	563.32	Joback Method
cpg	405.27	J/mol×K	597.44	Joback Method
cpg	421.05	J/mol×K	631.56	Joback Method

cpg	435.83	J/mol×K	665.68	Joback Method
cpg	449.76	J/mol×K	699.79	Joback Method
cpg	463.00	J/mol×K	733.91	Joback Method
cpg	475.71	J/mol×K	768.03	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=R485393&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume