3-methyl-1-adamantanol

Inchi: InChI=1S/C11H18O/c1-10-3-8-2-9(4-10)6-11(12,5-8)7-10/h8-9,12H,2-7H2,1H3
InchiKey: PJBDPRVLKHVTCY-UHFFFAOYSA-N
Formula: C11H18O
SMILES: CC12CC3CC(C1)CC(O)(C3)C2
Mol. weight [g/mol]: 166.26

Physical Properties

Property code	Value	Unit	Source
gf	56.38	kJ/mol	Joback Method
hf	-200.22	kJ/mol	Joback Method
hfus	9.11	kJ/mol	Joback Method
hvap	54.06	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.338		Crippen Method
mcvol	139.140	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpol	1317.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1305.00		NIST Webbook
ripol	1845.00		NIST Webbook
ripol	1863.00		NIST Webbook
ripol	1827.00		NIST Webbook
ripol	1827.00		NIST Webbook
tb	563.56	K	Joback Method
tc	776.36	K	Joback Method
tf	368.41	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.16	J/mol×K	563.56	Joback Method
cpg	403.85	J/mol×K	599.03	Joback Method

cpg	419.30	J/mol×K	634.49	Joback Method
cpg	433.76	J/mol×K	669.96	Joback Method
cpg	447.50	J/mol×K	705.42	Joback Method
cpg	460.76	J/mol×K	740.89	Joback Method
cpg	473.82	J/mol×K	776.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R304744&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