Adamantane-1,3-diol

Other names: 1,3-Dihydroxyadamantane
Inchi: InChI=1S/C10H16O2/c11-9-2-7-1-8(4-9)5-10(12,3-7)6-9/h7-8,11-12H,1-6H2
InchiKey: MOLCWHCSXCKHAP-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: OC12CC3CC(C1)CC(O)(C3)C2
Mol. weight [g/mol]: 168.23
CAS: 5001-18-3

Physical Properties

Property code	Value	Unit	Source
gf	-88.86	kJ/mol	Joback Method
hf	-331.81	kJ/mol	Joback Method
hfus	10.61	kJ/mol	Joback Method
hvap	68.51	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.062		Crippen Method
mcvol	130.920	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
rinpol	1473.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1473.00		NIST Webbook
tb	632.86	K	Joback Method
tc	834.37	K	Joback Method
tf	417.96	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.27	J/mol×K	632.86	Joback Method
cpg	407.93	J/mol×K	666.45	Joback Method

cpg	419.97	J/mol×K	700.03	Joback Method
cpg	431.59	J/mol×K	733.62	Joback Method
cpg	443.02	J/mol×K	767.20	Joback Method
cpg	454.48	J/mol×K	800.79	Joback Method
cpg	466.18	J/mol×K	834.37	Joback Method

Sources

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=C5001183&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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