5,7-Dimethyl-1,3-adamantanediol

Other names: 1,3-Dimethyladamantene-5,7-diol
1,3-Dimethyladamantane-5,7-diol
Inchi: InChI=1S/C12H20O2/c1-9-3-10(2)6-11(13,4-9)8-12(14,5-9)7-10/h13-14H,3-8H2,1-2H3
InchiKey: XNTKRLBGVHQKEJ-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: CC12CC3(C)CC(O)(C1)CC(O)(C2)C3
Mol. weight [g/mol]: 196.29
CAS: 10347-01-0

Physical Properties

Property code	Value	Unit	Source
gf	-83.00	kJ/mol	Joback Method
hf	-342.61	kJ/mol	Joback Method
hfus	3.20	kJ/mol	Joback Method
hvap	70.66	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	1.843		Crippen Method
mcvol	159.100	ml/mol	McGowan Method
pc	3791.65	kPa	Joback Method
rinpol	1484.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1461.00		NIST Webbook
tb	679.10	K	Joback Method
tc	888.61	K	Joback Method
tf	488.30	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.94	J/mol×K	679.10	Joback Method
cpg	502.67	J/mol×K	714.02	Joback Method

cpg	516.44	J/mol×K	748.94	Joback Method
cpg	530.63	J/mol×K	783.85	Joback Method
cpg	545.67	J/mol×K	818.77	Joback Method
cpg	561.95	J/mol×K	853.69	Joback Method
cpg	579.87	J/mol×K	888.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10347010&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume