1,3-Dimethyladamantane-5,7-diol

Other names: 1,3-Dimethyladamantane-5,7-diol
1,3-Dimethyladamantene-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

Physical Properties

Property code	Value	Unit	Source
hf	-499.25	kJ/mol	Cheméo Relay (1.0)
hfus	3.20	kJ/mol	Joback Method
ie	9.04	eV	Cheméo Relay (1.0)
logp	1.843		Crippen Method
mcvol	159.100	ml/mol	McGowan Method
rinpol	1438.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1484.00		NIST Webbook
tf	377.42	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10347010&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point