1,3-Dihydro-1-hydroxy-3,3-dimethyl-1(m-tolyl)-3,4

Inchi: InChI=1S/C17H18O2/c1-12-7-6-8-13(11-12)17(18)15-10-5-4-9-14(15)16(2,3)19-17/h4-11
InchiKey: XMLTURDDADEPER-UHFFFAOYSA-N
Formula: C17H18O2
SMILES: Cc1cccc(C2(O)OC(C)(C)c3ccccc32)c1
Mol. weight [g/mol]: 254.32
CAS: 7002-47-3

Physical Properties

Property code	Value	Unit	Source
gf	116.94	kJ/mol	Joback Method
hf	-145.38	kJ/mol	Joback Method
hfus	25.77	kJ/mol	Joback Method
hvap	77.80	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.454		Crippen Method
mcvol	203.750	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
tb	773.36	K	Joback Method
tc	1009.43	K	Joback Method
tf	508.12	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.61	J/mol×K	773.36	Joback Method
cpg	608.85	J/mol×K	812.70	Joback Method
cpg	625.15	J/mol×K	852.05	Joback Method
cpg	641.84	J/mol×K	891.39	Joback Method
cpg	659.23	J/mol×K	930.74	Joback Method
cpg	677.63	J/mol×K	970.08	Joback Method
cpg	697.35	J/mol×K	1009.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7002473&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume