«alpha»,«alpha»'-Dihydroxy-m-diisopropylbenzen

Other names: 1,3-Benzenedimethanol, «alpha»,«alpha»,«alpha»',«alpha»'-tetramethyl-
«alpha»,«alpha»,«alpha»',«alpha»'-tetramethyl-m-xylene-«alpha»,«alpha»'-diol
1,3-Di(2'-hydroxy isopropyl) benzene
Inchi: InChI=1S/C12H18O2/c1-11(2,13)9-6-5-7-10(8-9)12(3,4)14/h5-8,13-14H,1-4H3
InchiKey: UGPWRRVOLLMHSC-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: CC(C)(O)c1cccc(C(C)(C)O)c1
Mol. weight [g/mol]: 194.27
CAS: 1999-85-5

Physical Properties

Property code	Value	Unit	Source
gf	-115.02	kJ/mol	Joback Method
hf	-387.91	kJ/mol	Joback Method
hfus	13.84	kJ/mol	Joback Method
hvap	76.01	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.141		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
tb	683.52	K	Joback Method
tc	881.33	K	Joback Method
tf	390.42	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.07	J/mol×K	683.52	Joback Method
cpg	520.68	J/mol×K	848.36	Joback Method
cpg	511.48	J/mol×K	815.39	Joback Method
cpg	501.68	J/mol×K	782.42	Joback Method
cpg	491.22	J/mol×K	749.46	Joback Method
cpg	480.04	J/mol×K	716.49	Joback Method

cpg	529.35	J/mol×K	881.33	Joback Method
dvisc	0.0000104	Pa×s	683.52	Joback Method
dvisc	0.0000189	Pa×s	634.67	Joback Method
dvisc	0.0000382	Pa×s	585.82	Joback Method
dvisc	0.0000876	Pa×s	536.97	Joback Method
dvisc	0.0002371	Pa×s	488.12	Joback Method
dvisc	0.0008008	Pa×s	439.27	Joback Method
dvisc	0.0036683	Pa×s	390.42	Joback Method

Sources

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=C1999855&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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