2,2'-methylenebis[6-(1-methylcyclohexyl)-p-creso

Other names: Bis(2-hydroxy-5-methyl-3-[1-methylcyclohexyl]phenyl
Inchi: InChI=1S/C29H40O2/c1-20-15-22(26(30)24(17-20)28(3)11-7-5-8-12-28)19-23-16-21(2)1
InchiKey: PHXLONCQBNATSL-UHFFFAOYSA-N
Formula: C29H40O2
SMILES: Cc1cc(Cc2cc(C)cc(C3(C)CCCCC3)c2O)c(O)c(C2(C)CCCCC2)c1
Mol. weight [g/mol]: 420.63
CAS: 77-62-3

Physical Properties

Property code	Value	Unit	Source
gf	108.28	kJ/mol	Joback Method
hf	-430.21	kJ/mol	Joback Method
hfus	40.03	kJ/mol	Joback Method
hvap	111.93	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	7.749		Crippen Method
mcvol	361.970	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
tb	1137.02	K	Joback Method
tc	1410.57	K	Joback Method
tf	805.51	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1419.61	J/mol×K	1137.02	Joback Method
cpg	1467.30	J/mol×K	1182.61	Joback Method
cpg	1519.37	J/mol×K	1228.20	Joback Method
cpg	1576.47	J/mol×K	1273.79	Joback Method
cpg	1639.27	J/mol×K	1319.38	Joback Method
cpg	1708.43	J/mol×K	1364.98	Joback Method
cpg	1784.61	J/mol×K	1410.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77623&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume