Phenol, 4,4'-[thiobis(methylene)]bis[2,6-bis(1,1-dimethylet

Other names: «alpha»,«alpha»'-thiobis(2,6-di-tert-butyl-p-cresol)
bis-[3,5-di-tert-butyl-4-hydroxybenzyl]sulfide
Inchi: InChI=1S/C30H46O2S/c1-27(2,3)21-13-19(14-22(25(21)31)28(4,5)6)17-33-18-20-15-23(
InchiKey: UDFARPRXWMDFQU-UHFFFAOYSA-N
Formula: C30H46O2S
SMILES: CC(C)(C)c1cc(CSCc2cc(C(C)(C)C)c(O)c(C(C)(C)C)c2)cc(C(C)(C)C)c1O
Mol. weight [g/mol]: 470.75
CAS: 1620-93-5

Physical Properties

Property code	Value	Unit	Source
gf	123.26	kJ/mol	Joback Method
hf	-583.10	kJ/mol	Joback Method
hfus	46.02	kJ/mol	Joback Method
hvap	117.23	kJ/mol	Joback Method
log10ws	-9.11		Crippen Method
logp	8.721		Crippen Method
mcvol	414.130	ml/mol	McGowan Method
pc	1037.23	kPa	Joback Method
tb	1176.18	K	Joback Method
tc	1443.03	K	Joback Method
tf	798.30	K	Joback Method
vc	1.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1504.42	J/mol×K	1176.18	Joback Method
cpg	1534.31	J/mol×K	1220.66	Joback Method
cpg	1565.99	J/mol×K	1265.13	Joback Method
cpg	1599.90	J/mol×K	1309.61	Joback Method
cpg	1636.48	J/mol×K	1354.08	Joback Method
cpg	1676.15	J/mol×K	1398.56	Joback Method
cpg	1719.35	J/mol×K	1443.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1620935&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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