Phenol, 2,2'-thiobis[4-(1,1,3,3-tetramethylbutyl)-

Other names: 2,2'-Thiobis[4-(1,1,3,3-tetramethylbutyl)phenol]
Inchi: InChI=1S/C28H42O2S/c1-25(2,3)17-27(7,8)19-11-13-21(29)23(15-19)31-24-16-20(12-14
InchiKey: WQYFETFRIRDUPJ-UHFFFAOYSA-N
Formula: C28H42O2S
SMILES: CC(C)(C)CC(C)(C)c1ccc(O)c(Sc2cc(C(C)(C)CC(C)(C)C)ccc2O)c1
Mol. weight [g/mol]: 442.70
CAS: 3294-03-9

Physical Properties

Property code	Value	Unit	Source
gf	125.68	kJ/mol	Joback Method
hf	-518.88	kJ/mol	Joback Method
hfus	41.62	kJ/mol	Joback Method
hvap	111.46	kJ/mol	Joback Method
log10ws	-8.48		Crippen Method
logp	8.677		Crippen Method
mcvol	385.950	ml/mol	McGowan Method
pc	1203.12	kPa	Joback Method
tb	1120.46	K	Joback Method
tc	1383.14	K	Joback Method
tf	750.72	K	Joback Method
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1367.30	J/mol×K	1120.46	Joback Method
cpg	1393.92	J/mol×K	1164.24	Joback Method
cpg	1422.00	J/mol×K	1208.02	Joback Method
cpg	1451.96	J/mol×K	1251.80	Joback Method
cpg	1484.24	J/mol×K	1295.58	Joback Method
cpg	1519.24	J/mol×K	1339.36	Joback Method
cpg	1557.42	J/mol×K	1383.14	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3294039&Units=SI

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