4,4'-(THIODIMETHYLENE)BIS(2,6-DI-TERT-BUTYL

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]: 470.76

Physical Properties

Property code	Value	Unit	Source
hf	-513.83	kJ/mol	Cheméo Relay (1.0)
hfus	46.02	kJ/mol	Joback Method
hvap	150.27	kJ/mol	Cheméo Relay (1.0)
ie	7.37	eV	Cheméo Relay (1.0)
logp	8.721		Crippen Method
mcvol	414.130	ml/mol	McGowan Method
tb	663.58	K	Cheméo Relay (1.0)
tf	417.20 ± 0.50	K	NIST Webbook

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
hfust	43.10	kJ/mol	417.20	NIST Webbook

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1620935&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point