

Phenol, 4,4'-thiobis[2-(1,1-dimethylethyl)-6-methyl-

Other names:

o-Cresol, 4,4'-thiobis[6-tert-butyl-
Antioxidant E 736
Antioxidant 736
E 736
Ethyl Antioxidant 736
Ethyl 736
Thioalkofen BM
Tioalkofen BM
TB 2
3-tert-Butyl-4-hydroxy-5-methylphenyl sulfide
4,4'-Thiobis(6-tert-butyl-o-cresol)
o-Cresol, 4,4'-thiobis(6-t-butyl-
Ethanox 736
4,4'-Thiobis(2-tert-butyl-6-methylphenol)
NSC 58409
6,6'-di-tert-butyl-4,4'-thiodi-o-cresol

Inchi:

InChI=1S/C22H30O2S/c1-13-9-15(11-17(19(13)23)21(3,4)5)25-16-10-14(2)20(24)18(12-

InchiKey:

YFHKLSPMRRWLKI-UHFFFAOYSA-N

Formula:

C22H30O2S

SMILES:

Cc1cc(Sc2cc(C)c(O)c(C(C)(C)C)c2)cc(C(C)(C)C)c1O

Mol. weight [g/mol]:

358.54

CAS:

96-66-2

Physical Properties

Property code	Value	Unit	Source
gf	50.22	kJ/mol	Joback Method
hf	-400.48	kJ/mol	Joback Method
hfus	40.13	kJ/mol	Joback Method
hvap	102.02	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	6.461		Crippen Method
mcvol	301.410	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
tb	999.60	K	Joback Method
tc	1258.08	K	Joback Method
tf	703.30	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	979.30	J/mol×K	999.60	Joback Method
cpg	998.24	J/mol×K	1042.68	Joback Method
cpg	1017.35	J/mol×K	1085.76	Joback Method
cpg	1036.90	J/mol×K	1128.84	Joback Method
cpg	1057.17	J/mol×K	1171.92	Joback Method
cpg	1078.46	J/mol×K	1215.00	Joback Method
cpg	1101.03	J/mol×K	1258.08	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	589.20	K	5.30	NIST Webbook

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=C96662&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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