Santonox

Other names:

Phenol, 4,4'-thiobis[2-(1,1-dimethylethyl)-5-methyl-
m-Cresol, 4,4'-thiobis[6-tert-butyl-
Disperse MB-61
Santonox BM
Santowhite crystals
Santox
Sumilizer WX
Thioalkofen BM 4
Thioalkofen BMCh
Thioalkofen MBCh
Thioalkophene BM-4
Yoshinox SR
3-tert-Butyl-4-hydroxy-6-methylphenyl sulfide
4,4'-Thiobis(2-tert-butyl-5-methylphenol)
Bis(3-tert-butyl-4-hydroxy-6-methylphenyl) sulfide
Bis(4-hydroxy-5-tert-butyl-2-methylphenyl) sulfide
Sumilizer WX-R
USAF B-15
1,1'-Thiobis(2-methyl-4-hydroxy-5-tert-butylbenzene)
4,4'-Thiobis(3-methyl-6-tert-butylphenol)
4,4'-Thiobis(6-tert-butyl-m-cresol)
4,4'-Thiobis(6-tert-butyl-3-methylphenol)
Santonox R
Yoshinox S
5-t-Butyl-4-hydroxy-2-methylphenyl sulfide
4,4'-Thio-bis (2-t-butyl-5-methylphenol)
4,4-Thiobis-(6-t-butyl-3-methyl-phenol)
5-tert-Butyl-4-hydroxy-2-methylphenyl sulfide
Lowinox 44S36
Ultranox 236
4,4'-Thiobis(3-methyl-6-t-butylphenol)
Antage Crystal
Antioxidant AO
Antioxidant TMB 6
NSC 35388
Nocrac 300
Nonflex BPS
6,6'-di-tert-butyl-4,4'-thiodi-m-cresol

Inchi: InChI=1S/C22H30O2S/c1-13-9-17(23)15(21(3,4)5)11-19(13)25-20-12-16(22(6,7)8)18(24

InchiKey: HXIQYSLFEXIOAV-UHFFFAOYSA-N

Formula: C22H30O2S
SMILES: Cc1cc(O)c(C(C)(C)C)cc1Sc1cc(C(C)(C)C)c(O)cc1C
Mol. weight [g/mol]: 358.54
CAS: 96-69-5

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

Sources

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=C96695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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