Bithionol

Other names:	2,2'-Thiobis(4,6-dichlorophenol)
	Phenol, 2,2'-thiobis[4,6-dichloro-
	Actamer
	Bidiphen
	Bis(2-hydroxy-3,5-dichlorophenyl) sulfide
	Bisoxyphen
	Bithin
	Bithional
	Bithionolate
	Bitin
	Bitionol
	CP 3438
	D 26
	Lorothidol
	Lorothiodol
	Neopellis
	Nobacter
	TBP
	USAF B-22
	Vancide BL
	XL 7
	2-Hydroxy-3,5-dichlorophenyl sulfide
	2,2'-Dihydroxy-3,3',5,5'-tetrachlorodiphenyl sulfide
	Bis(3,5-dichloro-2-hydroxyphenyl) sulfide
	Bithionol sulfide
	2-Hydroxy-3,5-dichlorophenyl sulphide
	NCI-C60628
	NSC 47129
	TKhSD
Inchi:	InChI=1S/C12H6Cl4O2S/c13-5-1-7(15)11(17)9(3-5)19-10-4-6(14)2-8(16)12(10)18/h1-4,1
InchiKey:	JFIOVJDNOJYLKP-UHFFFAOYSA-N
Formula:	C12H6Cl4O2S
SMILES:	Oc1c(Cl)cc(Cl)cc1Sc1cc(Cl)cc(Cl)c1O
Mol. weight [g/mol]:	356.05
CAS:	97-18-7

Physical Properties

Property code	Value	Unit	Source
gf	-87.38	kJ/mol	Joback Method
hf	-239.54	kJ/mol	Joback Method
hfus	45.85	kJ/mol	Joback Method
hvap	99.89	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	5.863		Crippen Method
mcvol	209.470	ml/mol	McGowan Method
pc	3901.37	kPa	Joback Method
tb	926.98	K	Joback Method
tc	1215.98	K	Joback Method
tf	705.44	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.71	J/mol×K	926.98	Joback Method
cpg	488.88	J/mol×K	975.15	Joback Method
cpg	498.37	J/mol×K	1023.31	Joback Method
cpg	508.41	J/mol×K	1071.48	Joback Method
cpg	519.25	J/mol×K	1119.65	Joback Method
cpg	531.14	J/mol×K	1167.81	Joback Method
cpg	544.30	J/mol×K	1215.98	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C97187&Units=SI

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

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