

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	m ³ /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

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

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

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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

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