

Fenticlor

Other names:

Bis(2-hydroxy-5-chlorophenyl) sulfide
Phenol, 2,2'-thiobis[4-chloro-
CR 305
D 25
D 25-Antimykotikum
Fenticlor
HL 1050
Meflorin
Novex
Oksid
Ovitrol
Ph 549
S 7 (antimycotic)
S 7
2,2'-Dihydroxy-5,5'-dichlorodiphenyl sulfide
2,2'-Dihydroxy-5,5'-dichlorophenyl sulfide
2,2'-Thiobis(4-chlorophenol)
5,5'-Dichloro-2,2'-dihydroxydiphenyl sulfide
NSC-4112
NSC 55636

Inchi:

InChI=1S/C12H8Cl2O2S/c13-7-1-3-9(15)11(5-7)17-12-6-8(14)2-4-10(12)16/h1-6,15-16H

InchiKey:

ANUSOIHIIPAHJV-UHFFFAOYSA-N

Formula:

C₁₂H₈Cl₂O₂S

SMILES:

Oc1ccc(Cl)cc1Sc1cc(Cl)ccc1O

Mol. weight [g/mol]:

287.16

CAS:

97-24-5

Physical Properties

Property code	Value	Unit	Source
gf	-44.26	kJ/mol	Joback Method
hf	-185.12	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	89.80	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.556		Crippen Method
mcvol	184.990	ml/mol	McGowan Method
pc	4462.28	kPa	Joback Method

tb	842.16	K	Joback Method
tc	1129.31	K	Joback Method
tf	620.56	K	Joback Method
vc	0.576	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.84	J/mol×K	842.16	Joback Method
cpg	460.70	J/mol×K	890.02	Joback Method
cpg	470.43	J/mol×K	937.88	Joback Method
cpg	480.27	J/mol×K	985.73	Joback Method
cpg	490.48	J/mol×K	1033.59	Joback Method
cpg	501.31	J/mol×K	1081.45	Joback Method
cpg	513.03	J/mol×K	1129.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97245&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

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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