2,2'-THIOBIS(4-CHLOROPHENOL)

Other names: Bis(2-hydroxy-5-chlorophenyl) sulfide
Phenol, 2,2'-thiobis[4-chloro-
CR 305
D 25
D 25-Antimykotikum
Fentichlor
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]: 287.17

Physical Properties

Property code	Value	Unit	Source
hf	-174.91	kJ/mol	Cheméo Relay (1.0)
hfus	38.23	kJ/mol	Joback Method
hvap	116.74	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.74		Cheméo Relay (1.0)
logp	4.556		Crippen Method
mcvol	184.990	ml/mol	McGowan Method
tb	612.55	K	Cheméo Relay (1.0)
tf	424.95	K	Cheméo Relay (1.0)

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C97245&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
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
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

Latest version available from: