Captafol

Other names: (Tetrachloroethylthio)tetrahydrophthalimide
3a,4,7,7a-Tetrahydro-2-[(1,1,2,2-tetrachloroethyl)thio]-1H-isoindole-1,3(2H)-dione
4-Cyclohexene-1,2-dicarboximide, N-[(1,1,2,2-tetrachloroethyl)thio]-
Alfloc 7020
Alfloc 7046
Arborseal
CS 5623
Captatol
Captofol
Difolatan
Difolatan 4F
Difolatan 4F1
Difolatan 80W
Difolatan BOW
Difosan
Folcid
Foltaf
Haipen 50
Merpafol
N-((1,1,2,2-Tetrachloroethyl)sulfenyl)-cis-4-cyclohexene-1,2-dicarboximide
N-(1,1,2,2-Tetrachloraethylthio)-cyclohex-4-en-1,4-diacarboximid
N-(1,1,2,2-Tetrachloraethylthio)-tetrahydrophthalamid
N-(1,1,2,2-Tetrachloroethylthio)-4-cyclohexene-1,2-dicarboximide
N-(1,1,2,2-Tetrachloroethylthio)-«DELTA»4-tetrahydrophthalimide
N-(1,1,2,2-Tetrachloroethylthio)-Â«DELTAÂ»4-tetrahydrophthalimide
N-(Tetrachloroethylthio)tetrahydrophthalimide
N-1,1,2,2-Tetrachloroethylmercapto-4-cyclohexene-1,2-carboximide
Nalco 7046
Ortho 5,865
Ortho 5865
Proxel EF
Sanspor
Santar SM
Sulfonimide
Sulpheimide
Terrazol

Inchi: InChI=1S/C10H9Cl4NO2S/c11-9(12)10(13,14)18-15-7(16)5-3-1-2-4-6(5)8(15)17/h1-2,5-6

InchiKey: JHRWWRDRBPCWTF-UHFFFAOYSA-N

Formula: C10H9Cl4NO2S

SMILES: O=C1C2CC=CCC2C(=O)N1SC(Cl)(Cl)C(Cl)Cl

Mol. weight [g/mol]: 349.06
CAS: 2425-06-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Estimated Solubility Method
logp	3.521		Crippen Method
mcvol	204.170	ml/mol	McGowan Method
tf	432.81 ± 0.20	K	NIST Webbook
tf	432.00 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	40.22	kJ/mol	432.70	NIST Webbook
hfust	43.10	kJ/mol	432.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2425061&Units=SI

Legend

hfust: Enthalpy of fusion at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point