Cis-captafol

Other names: 1H-Isoindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-2-[(1,1,2,2-tetrachloroethyl)thio]-, cis-
4-Cyclohexene-1,2-dicarboximide, N-[(1,1,2,2-tetrachloroethyl)thio]-, cis-
N-(1,1,2,2-Tetrachloro-ethylsulfenyl)cis-4-cyclohexene-1,2-dicarboximide
TN 80
Crisfolatan
Mycodifol
Pillartan
cis-N-((1,1,2,2-Tetrachloroethyl)thio)-4-cyclohexene-1,2-dicarboxymide
cis-3a,4,7,7a-Tetrahydro-2-((1,1,2,2-tetrachloroethyl)thio)-1H-isoindole-1,3(2H)-dione
N-(Tetrachloroethylthio)-«DELTA»4-tetrahydrophthalimide
Captafol, cis-
1H-Isoindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-2-((1,1,2,2-tetrachloroethyl)thio)-, (3aR,7aS)-rel-
TN 80 (pesticide)
cis-N-((1,1,2,2-Tetrachloroethyl)thio)-4-cyclohexene-1,2-dicarboximide

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-OLQVQODUSA-N

Formula: C10H9Cl4NO2S

SMILES: O=C1[C@H]2CC=CC[C@H]2C(=O)N1SC(Cl)(Cl)C(Cl)Cl

Mol. weight [g/mol]: 349.07

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.15		Cheméo Relay (1.0)
logp	3.521		Crippen Method
mcvol	204.170	ml/mol	McGowan Method
tf	415.94	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2939802&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

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