

Captan

Other names:

1H-Isoindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-2-[(trichloromethyl)thio]-
4-Cyclohexene-1,2-dicarboximide, N-[(trichloromethyl)thio]-
Aacaptan
Amercide
Captaf
Captaf 85W
Captan 50W
Captex
Esso fungicide 406
Flit 406
Fungus Ban Type II
Glyodex 37-22
Kaptan
Malipur
N-[(Trichloromethyl)thio]tetrahydrophthalimide
N-Trichloromethylthio-3a,4,7,7a-tetrahydrophthalimide
Neracid
Orthocide
Orthocide 406
Orthocide 50
Orthocide 7.5
Orthocide 75
Orthocide 83
Ortocid 50
Stauffer captan
SR 406
Vancide 89
Vancide 89RE
Vanguard K
Captane
ENT 26,538
Le captane
Merpan
N-((Trichloromethyl)mercapto)-«DELTA»4-tetrahydrophthalimide
N-((Trichloromethyl)mercapto)-4-cyclohexene-1,2-dicarboximide
N-((Trichloromethyl)thio)-4-cyclohexene-1,2-dicarboximide
N-((Trichloromethyl)thio)cyclohex-4-ene-1,2-dicarboximide
NCI-C00077
Vondcaptan
Agrosol S

Agrox 2-way and 3-way
 Bangton
 Bean seed protectant
 Captab
 Captancapteneet 26,538
 Captan-streptomycin 7.5-0.1 potato seed piece protectant
 Granox PFM
 Gustafson captan 30-dd
 Hexacap
 Micro-check 12
 Osocide
 3a,4,7,7a-Tetrahydro-N-(trichloromethanesulphenyl)phthalimide
 1,2,3,6-Tetrahydro-N-(trichloromethylthio)phthalimide
 Trichlormethylthioamid kyseliny 1,2,3,6-tetrahydroftalove
 N-(Trichlor-methylthio)-phthalimid
 Trichloromethylthio-1,2,5,6-tetrahydrophthalamide
 Vancide P-75
 Vanguard K
 Vanicide
 N-[(Trichloromethyl)thio]-«DELTA»4-tetrahydrophthalimide
 Trimegol
 3a,4,7,7a-Tetrahydro-2-[(trichloromethyl)thio]-1H-isoindole-1,3(2H)dione
 N-Trichloromethyl-thio-3a,4,7,7a-tetrahydrophthalimide
 Venturin
 Deltan
 Bangtan
 Kaptazor
 Zenecal
 Ugecap
 Orthocide S 50

Inchi: InChI=1S/C9H8Cl3NO2S/c10-9(11,12)16-13-7(14)5-3-1-2-4-6(5)8(13)15/h1-2,5-6H,3-4H
InchiKey: LDVVMCZRFBWMZSG-UHFFFAOYSA-N
Formula: C9H8Cl3NO2S
SMILES: O=C1C2CC=CCC2C(=O)N1SC(Cl)(Cl)Cl
Mol. weight [g/mol]: 300.59
CAS: 133-06-2

Physical Properties

Property code	Value	Unit	Source
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log10ws	-3.80		Crippen Method
logp	2.913		Crippen Method
mcvol	177.840	ml/mol	McGowan Method
rinpol	2075.00		NIST Webbook
rinpol	2019.00		NIST Webbook
rinpol	2079.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	2019.00		NIST Webbook
tf	447.10 ± 0.20	K	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C133062&Units=SI

Legend

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

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