

Coumaphos

Other names:

3-Chloro-4-methyl-7-coumarinyl diethyl phosphorothioate
3-Chloro-4-methyl-7-hydroxycoumarin diethyl thiophosphoric acid ester
3-Chloro-4-methylumbelliferone O-ester with O,O-diethyl phosphorothioate
3-Chloro-7-hydroxy-4-methyl-coumarin O,O-diethyl phosphorothioate
3-Chloro-7-hydroxy-4-methyl-coumarin O-ester with O,O-diethyl phosphorothioate
3-chloro-7-diethoxyphosphinothioxyloxy-4-methylchromen-2-one
Agridip
Asunthol
Asuntol
Azunthol
BAY 21/199
Bayer 21/199
Baymix
Baymix 50
Co-ral
Co-ral (Coumaphos)
Co-ral (phosphate)
Coumafos
Coumarin, 3-chloro-7-hydroxy-4-methyl-, O-ester with O,O-diethyl phosphorothioate
Cumafos
Diethyl 3-chloro-4-methylumbelliferyl thionophosphate
Diethyl thiophosphoric acid ester of 3-chloro-4-methyl-7-hydroxycoumarin
Diolice
ENT 17,957
Koral
Meldane
Meldone
Muscatox
NA 2783
NCI-C08662
Negashunt
O,O-Diaethyl-O-(3-chlor-4-methyl-coumarin-7-yl)-monothiophosphat
O,O-Diethyl 3-chloro-4-methyl-7-umbelliferone thiophosphate
O,O-Diethyl O-(3-chloro-4-methyl-2-oxo-2H-1-benzopyran-7-yl)phosphorothioate
O,O-Diethyl O-(3-chloro-4-methyl-2-oxo-2H-benzopyran-7-yl)phosphorothioate
O,O-Diethyl O-(3-chloro-4-methyl-7-coumarinyl)phosphorothioate
O,O-Diethyl O-(3-chloro-4-methylcoumarinyl-7) thiophosphate
O,O-Diethyl O-(3-chloro-4-methylumbelliferyl)phosphorothioate
O,O-Diethyl-O-(3-chloor-4-methyl-coumarin-7-yl)monothiofosfaat
O,O-Diethyl-O-(3-chloro-4-methyl-coumarin-7-yl)monothiofosfaat

O,O-Dietil-O-(3-chloro-4-metil-cumarin-7-il-monotiofosfato)
 O,O-Dietil-O-(3-cloro-4-metil-cumarin-7-il-monotiofosfato)
 O-(3-Chloro-4-methyl-2-oxo-2H-1-benzopyran-7-yl) O,O-diethyl phosphorothioate
 O-(3-Chloro-4-methylcoumarin-7-yl) O,O-diethyl phosphorothioate
 O-3-Chloro-4-methyl-7-coumarinyl O,O-diethyl phosphorothioate
 OMS 485
 Perizin
 Phosphorothioic acid, O,O-diethyl ester, O-ester with
 3-chloro-7-hydroxy-4-methylcoumarin
 Phosphorothioic acid, O-(3-chloro-4-methyl-2-oxo-2H-1-benzopyran-7-yl)
 O,O-diethyl ester
 Resistox
 Resitox
 Suntol
 Thiophosphate de O,O-diethyle et de O-(3-chloro-4-methyl-7-coumarinyle)
 Umbethion

Inchi: InChI=1S/C14H16ClO5PS/c1-4-17-21(22,18-5-2)20-10-6-7-11-9(3)13(15)14(16)19-12(11)
InchiKey: BXNANOICGRISHX-UHFFFAOYSA-N
Formula: C14H16ClO5PS
SMILES: CCOP(=S)(OCC)Oc1ccc2c(C)c(Cl)c(=O)oc2c1
Mol. weight [g/mol]: 362.77
CAS: 56-72-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.62		Aqueous Solubility Prediction Method
log10ws	-5.38		Estimated Solubility Method
logp	4.431		Crippen Method
mcvol	243.300	ml/mol	McGowan Method
rinsol	2654.00		NIST Webbook
rinsol	2654.00		NIST Webbook
tf	368.40 ± 0.10	K	NIST Webbook

Sources

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=C56724&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

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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