

Carbophenothion

Other names:

(4-chlorophenyl)sulfanylmethylsulfanyl-diethoxy-sulfanylidene phosphorane
Acarithion
Akarithion
Carbofenothion
Carbofenotion
Carbofenthion
Carbophenthion
Dagadip
Dithiophosphate de O,O-diethyle et de (4-chloro-phenyl) thiomethyle
Endyl
Ethyl carbophenothion
Garrathion
Hexathion
Karbofenothion
Lethox
NSC 231691
Nephocarp
O,O-Diaethyl-S-((4-chlor-phenyl-thio)methyl)dithiophosphat
O,O-Diethyl (((p-chlorophenyl)mercapto)methyl) dithiophosphate
O,O-Diethyl S-(((4-chlorophenyl)thio)methyl) dithiophosphate
O,O-Diethyl S-(((p-chlorophenyl)thio)methyl) dithiophosphate
O,O-Diethyl S-(p-Chlorophenylthio)methyl phosphorodithioate
O,O-Diethyl dithiophosphoric acid p-chlorophenylthiomethyl ester
O,O-Diethyl-S-p-chlorfenylthiomethylester kyseliny dithiofosforecne
OMS 244
Oleoakarithion
Phosphorodithioic acid, S-[[[4-chlorophenyl]thio]methyl] O,O-diethyl ester
Phosphorodithioic acid, S-[[[p-chlorophenyl]thio]methyl] O,O-diethyl ester
S-(((4-Chlorophenyl)thio)methyl)diethyl phosphorothiolothionate
S-(4-Chlorophenylthiomethyl) OO-diethyl phosphorodithioate
S-[[[p-Chlorophenyl]thio]methyl] O,O-diethyl phosphorodithioate
Stauffer R-1,303
Stauffer R-1303
Trithion
Trithion miticide
Trithiontylphenol

Inchi: InChI=1S/C11H16ClO2PS3/c1-3-13-15(16,14-4-2)18-9-17-11-7-5-10(12)6-8-11/h5-8H,3-
InchiKey: VEDTXTNSFWUXGQ-UHFFFAOYSA-N
Formula: C11H16ClO2PS3
SMILES: CCOP(=S)(OCC)SCSc1ccc(Cl)cc1

Mol. weight [g/mol]: 342.87
CAS: 786-19-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.87		Aqueous Solubility Prediction Method
log10ws	-5.74		Estimated Solubility Method
logp	5.420		Crippen Method
mcvol	235.580	ml/mol	McGowan Method
rinpol	2277.00		NIST Webbook
rinpol	2337.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2255.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2244.00		NIST Webbook
rinpol	2255.00		NIST Webbook
ripol	3306.00		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=C786196&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
ripol: Polar retention indices

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