

Carbophenothion sulfone

Other names:

Phosphorodithioic acid, S-[[[(4-chlorophenyl)sulfonyl]methyl] O,O-diethyl ester
Phosphorodithioic acid, S-[[[(p-chlorophenyl)sulfonyl]methyl] O,O-diethyl ester
O,O-Diethyl S-(p-chlorophenylsulfonyl)methyl phosphorodithioate
R 1776

Inchi:

S-p-Chlorophenylsulfonylmethyl O,O-diethyl phosphorodithioate

InchiKey:

InChI=1S/C11H16ClO4PS3/c1-3-15-17(18,16-4-2)19-9-20(13,14)11-7-5-10(12)6-8-11/h5

Formula:

CBXRYOZUHFXMRF-UHFFFAOYSA-N

SMILES:

C11H16ClO4PS3

Mol. weight [g/mol]:

CCOP(=S)(OCC)SCS(=O)(=O)c1ccc(Cl)cc1

CAS:

374.86

16662-85-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.33		Crippen Method
logp	4.102		Crippen Method
mcvol	247.320	ml/mol	McGowan Method

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.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=C16662854&Units=SI>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

mcvol:

McGowan's characteristic volume

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