

Carbophenoxon sulfone

Other names:

Phosphorothioic acid, S-[[[(4-chlorophenyl)sulfonyl]methyl] O,O-diethyl ester
Phosphorothioic acid, S-[[[(p-chlorophenyl)sulfonyl]methyl] O,O-diethyl ester
Methanethiol, [(p-chlorophenyl)sulfonyl]-, S-ester with O,O-diethyl phosphorothioate
O,O-Diethyl S-(p-chlorophenylsulfonyl)methyl phosphorothioate
R 1777
S-(p-Chlorophenylsulfonyl)methyl O,O-diethyl phosphorothioate
Carbophenothion oxon sulfone
Trithion oxon sulfone
S-([(4-Chlorophenyl)sulfonyl]methyl) O,O-diethyl thiophosphate
Carbophenothion O-analog sulfone

Inchi:

InChI=1S/C11H16ClO5PS2/c1-3-16-18(13,17-4-2)19-9-20(14,15)11-7-5-10(12)6-8-11/h5

InchiKey:

AQORIFUYBMSEHZ-UHFFFAOYSA-N

Formula:

C11H16ClO5PS2

SMILES:

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

Mol. weight [g/mol]:

358.80

CAS:

16662-87-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.34		Crippen Method
logp	3.986		Crippen Method
mcpvol	236.840	ml/mol	McGowan Method

Sources

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=C16662876&Units=SI>

Crippen Method:

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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/60-912-2/Carbophenoxon-sulfone.pdf>

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