

Carbophenoxon sulfoxide

Other names:

Phosphorothioic acid, S-[[[(4-chlorophenyl)sulfinyl]methyl] O,O-diethyl ester
Phosphorothioic acid, S-[[[(p-chlorophenyl)sulfinyl]methyl] O,O-diethyl ester
O,O-Diethyl S-(p-chlorophenylsulfinyl)methyl phosphorothioate
R 1990
S-p-Chlorophenylsulfinylmethyl O,O-diethyl phosphorothioate
Carbophenothion O-analog sulfoxide

Inchi:

InChI=1S/C11H16ClO4PS2/c1-3-15-17(13,16-4-2)18-9-19(14)11-7-5-10(12)6-8-11/h5-8H

InchiKey:

XQKGIZXBDUMZBY-UHFFFAOYSA-N

Formula:

C11H16ClO4PS2

SMILES:

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

Mol. weight [g/mol]:

342.80

CAS:

16662-86-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Crippen Method
logp	4.319		Crippen Method
mcvol	230.970	ml/mol	McGowan Method

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C16662865&Units=SI>

Crippen Method:

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

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

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/118-640-0/Carbophenoxon-sulfoxide.pdf>

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