

prothiofos

Other names:

Prothiophos
Phosphorodithioic acid, O-(2,4-dichlorophenyl) O-ethyl S-propyl ester
Tokuthion
Prothiofos
Bay NTN 8629
Bideron

o-(2,4-Dichlorophenyl) o-ethyl S-propyl phosphorodithioate

O-(2,4-dichlorophenyl) O-ethyl S-propyl dithiophosphate

Inchi: InChI=1S/C11H15Cl2O2PS2/c1-3-7-18-16(17,14-4-2)15-11-6-5-9(12)8-10(11)13/h5-6,8H

InchiKey: FITIWKDOCAUBQD-UHFFFAOYSA-N

Formula: C11H15Cl2O2PS2

SMILES: CCCSP(=S)(OCC)Oc1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 345.25

CAS: 64772-54-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.86		Crippen Method
logp	5.776		Crippen Method
mcvol	231.470	ml/mol	McGowan Method
rinpol	2093.00		NIST Webbook
rinpol	2095.00		NIST Webbook
rinpol	2120.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2170.00		NIST Webbook
rinpol	2129.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2093.00		NIST Webbook
rinpol	2129.00		NIST Webbook
rinpol	2170.00		NIST Webbook
rinpol	2120.00		NIST Webbook
rinpol	2101.00		NIST Webbook
ripol	2915.00		NIST Webbook
ripol	2915.00		NIST Webbook

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=C34643464&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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