

Pyraclofos

Other names:	Thiophosphoric acid, O-[1-(4-chlorophenyl)-1H-pyrazol-4-yl] ester, O,-ethyl ester, S-propyl ester 1-(4-Chlorophenyl)-4-(ethoxy-propylsulfanyl-phosphoryl)oxy-pyrazole O-[1-(4-Chlorophenyl)-1H-pyrazol-4-yl] O-ethyl S-propyl phosphorothioate Phosphorothioic acid, O-[1-(4-chlorophenyl)-1H-pyrazol-4-yl] O-ethyl S-propyl ester Starlet Boltage
Inchi:	InChI=1S/C14H18ClN2O3PS/c1-3-9-22-21(18,19-4-2)20-14-10-16-17(11-14)13-7-5-12(1
InchiKey:	QHGVXILFMXYDRS-UHFFFAOYSA-N
Formula:	C14H18ClN2O3PS
SMILES:	CCCSP(=O)(OCC)Oc1cnn(-c2ccc(Cl)cc2)c1
Mol. weight [g/mol]:	360.80
CAS:	77458-01-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.60		Crippen Method
logp	5.192		Crippen Method
mcvol	251.520	ml/mol	McGowan Method
rinpol	2687.00		NIST Webbook
rinpol	2660.00		NIST Webbook
rinpol	2664.00		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=C77458016&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcpol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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