Cyanophenphos

Other names:	Phosphonothioic acid, phenyl-, O-(4-cyanophenyl) O-ethyl ester Phosphonothioic acid, phenyl-, O-ethyl ester, O-ester with p-hydroxybenzonitrile B 10094 Cyanofenphos CP 19699 CYP Monsanto CP-19699 O-Ethyl O-(4-cyanophenyl) phenylphosphonothioate OMS 870 S 4087 Surazon Surecide Benzonitrile, p-hydroxy-, O-ester with O-ethyl phenylphosphonothioate O-p-Cyanophenyl O-ethyl phenyl-phosphonothioate O-(4-Cyanophenyl) O-ethyl phenylphosphonothioate ENT 25,832 ENT 25,832-a O-Ethyl phenylphosphonothioate, O-ester with p-hydroxybenzonitrile Experimental insecticide S-4087 Phenylphosphonothioic acid O-ethyl ester O-ester with p-hydroxybenzonitrile Stauffer B-10094 Upjohn U-32714
Inchi:	InChI=1S/C15H14NO2PS/c1-2-17-19(20,15-6-4-3-5-7-15)18-14-10-8-13(12-16)9-11-14/h
InchiKey:	LRNJHZNPJSPMGK-UHFFFAOYSA-N
Formula:	C15H14NO2PS
SMILES:	CCOP(=S)(Oc1ccc(C#N)cc1)c1ccccc1
Mol. weight [g/mol]:	303.32
CAS:	13067-93-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.71		Crippen Method
logp	3.609		Crippen Method
mcvol	224.620	ml/mol	McGowan Method
rinpol	2236.00		NIST Webbook
rinpol	2260.00		NIST Webbook

rinpol	2245.00	NIST Webbook
rinpol	2243.00	NIST Webbook
rinpol	2252.00	NIST Webbook
rinpol	2243.00	NIST Webbook
rinpol	2268.00	NIST Webbook
rinpol	2252.00	NIST Webbook
rinpol	2260.00	NIST Webbook
rinpol	2268.00	NIST Webbook
rinpol	2245.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13067931&Units=SI
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

Legend

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

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