

Isoxathion

Other names:

Phosphorothioic acid, O,O-diethyl O-(5-phenyl-3-isoxazolyl) ester
O,O-Diethyl O-(5-phenyl-3-isoxazolyl) phosphorothioate
O,O-Diethyl O-(3-(5-phenyl)-1,2-isoxazolyl)phosphorothionate
E-48
Kaphos
SI-6711

O,O-Diethyl-O-(5-phenylisoxazol-3-yl) thiophosphate

O,O-diethyl O-5-phenylisoxazol-3-ylphosphorothioate

Inchi: InChI=1S/C13H16NO4PS/c1-3-15-19(20,16-4-2)18-13-10-12(17-14-13)11-8-6-5-7-9-11/h**InchiKey:** SDMSCIWHRZJSRN-UHFFFAOYSA-N**Formula:** C13H16NO4PS**SMILES:** CCOP(=S)(OCC)Oc1cc(-c2ccccc2)on1**Mol. weight [g/mol]:** 313.31**CAS:** 18854-01-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.38		Crippen Method
logp	4.018		Crippen Method
mcvol	221.080	ml/mol	McGowan Method
rinpol	2168.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2145.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2160.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>**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=C18854018&Units=SI>

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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