

Phosmet oxon

Other names:	Phosphorothioic acid, S-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl] O,O-dimethyl ester Phosphorothioic acid, O,O-dimethyl ester, S-ester with N-(mercaptomethyl)phthalimide N-(Mercaptomethyl)phthalimide S-(O,O-dimethylphosphorothioate) Imidoxon O,O-Dimethyl S-phthalimidomethyl phosphorothioate O,O-Dimethylphosphorothioate S-ester with N-(mercaptomethyl)phthalimide Oxoimidan R 1571 R 1571A R-1,571 S-Phthalimidomethyl O,O-Dimethyl phosphorothioate Stauffer R-1,571 Stauffer R-1571 Stauffer R-1571A 1H-Isoindole-1,3(2H)-dione, 2-[[[(dimethoxyphosphono)thio]methyl]-S-((1,3-Dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl) O,O-dimethyl phosphorothioate ENT 25,707 Imidan oxon Phosphorothioic acid, O,O-dimethyl S-phthalimidomethyl ester
Inchi:	InChI=1S/C11H12NO5PS/c1-16-18(15,17-2)19-7-12-10(13)8-5-3-4-6-9(8)11(12)14/h3-6H
InchiKey:	BEMXOWRVWRNPPL-UHFFFAOYSA-N
Formula:	C11H12NO5PS
SMILES:	<chem>COP(=O)(OC)SCN1C(=O)c2ccccc2C1=O</chem>
Mol. weight [g/mol]:	301.25
CAS:	3735-33-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.48		Crippen Method
logp	2.374		Crippen Method
mvol	198.770	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3735339&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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