

Phosphoric acid, dimethyl 3-methyl-4-nitrophenyl ester

Other names:	Accothion O-analog BAY 42247 m-Cresol, 4-Nitro-, dimethyl phosphate Dimethyl 4-nitro-m-tolyl phosphate Fenitrooxon Fenitrooxone Fenitrothion oxon Fenitrothion oxygen analog Metaoxon Oxo-Sumithion Phosphoric acid, dimethyl 4-nitro-m-tolyl ester Sumioxon Sumioxone O,O-Dimethyl O-(3-methyl-4-nitrophenyl)phosphate Fenitroxon 3-Methyl-4-nitrophenyl dimethyl phosphate Fenitrothion O-analog 3-Methyldimethylparaoxon O,O-Dimethyl O-(3-methyl-4-nitrophenyl)phosphorate
Inchi:	InChI=1S/C9H12NO6P/c1-7-6-8(4-5-9(7)10(11)12)16-17(13,14-2)15-3/h4-6H,1-3H3
InchiKey:	MJNAIAPNXYJWCT-UHFFFAOYSA-N
Formula:	C9H12NO6P
SMILES:	<chem>COP(=O)(OC)Oc1ccc([N+](=O)[O-])c(C)c1</chem>
Mol. weight [g/mol]:	261.17
CAS:	2255-17-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.57		Crippen Method
logp	2.683		Crippen Method
mcvol	175.270	ml/mol	McGowan Method
rinpol	1871.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1800.00		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=C2255176&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
rinpola:	Non-polar retention indices

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