

Phosphoric acid, dimethyl 4-nitrophenyl ester

Other names:	Phosphoric acid, dimethyl p-nitrophenyl ester BAY 11678 Dimethyl p-Nitrophenyl phosphate Dimethyl paraoxon Dimethyl 4-nitrophenyl phosphate Methyl-E 600 Methylparaoxon Paraoxon methyl Desmethylnitrophos O,O-Dimetyl-O-p-nitrofenylfosfat Dimethyl-p-nitrofenylester kyseliny fosforecne
Inchi:	InChI=1S/C8H10NO6P/c1-13-16(12,14-2)15-8-5-3-7(4-6-8)9(10)11/h3-6H,1-2H3
InchiKey:	BAFQDKPKJOLXFZ-UHFFFAOYSA-N
Formula:	C8H10NO6P
SMILES:	<chem>COP(=O)(OC)Oc1ccc([N+](=O)[O-])cc1</chem>
Mol. weight [g/mol]:	247.14
CAS:	950-35-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.10		Crippen Method
logp	2.374		Crippen Method
mcvol	161.180	ml/mol	McGowan Method
rinpol	1810.00		NIST Webbook
rinpol	1817.00		NIST Webbook
ripol	2737.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C950356&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
ripol:	Polar retention indices

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