

Phosphoric acid, 4-methoxyphenyl dimethyl ester

Other names:	Dimethyl 4-methoxyphenyl phosphate
Inchi:	InChI=1S/C9H13O5P/c1-11-8-4-6-9(7-5-8)14-15(10,12-2)13-3/h4-7H,1-3H3
InchiKey:	PHQVYYOBMMIRNS-UHFFFAOYSA-N
Formula:	C9H13O5P
SMILES:	<chem>COc1ccc(OP(=O)(OC)OC)cc1</chem>
Mol. weight [g/mol]:	232.17
CAS:	7357-14-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	2.475		Crippen Method
mcvol	163.720	ml/mol	McGowan Method
rinpol	1637.00		NIST Webbook
ripol	2350.00		NIST Webbook
ripol	2350.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7357144&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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