

Phosphorous acid, cyclic o-phenylene-, methyl ester

Inchi:	InChI=1S/C7H7O3P/c1-8-11-9-6-4-2-3-5-7(6)10-11/h2-5H,1H3
InchiKey:	WSJGYLOBOBYMCY-UHFFFAOYSA-N
Formula:	C7H7O3P
SMILES:	COP1Oc2ccccc2O1
Mol. weight [g/mol]:	170.10
CAS:	20570-25-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.90		Crippen Method
logp	2.331		Crippen Method
mcvol	112.940	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=C20570256&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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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