

Phosphorous acid, cyclic o-phenylene-, isobutyl ester

Inchi:	InChI=1S/C10H13O3P/c1-8(2)7-11-14-12-9-5-3-4-6-10(9)13-14/h3-6,8H,7H2,1-2H3
InchiKey:	HZAUOUTUWDZSGV-UHFFFAOYSA-N
Formula:	C10H13O3P
SMILES:	CC(C)COP1Oc2ccccc2O1
Mol. weight [g/mol]:	212.18
CAS:	4591-39-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.11		Crippen Method
logp	3.357		Crippen Method
mcvol	155.210	ml/mol	McGowan Method

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=C4591393&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/26-619-6/Phosphorous-acid-cyclic-o-phenylene-isobutyl-ester.pdf>

Generated by Cheméo on 2024-04-29 10:46:42.000121201 +0000 UTC m=+16676850.920698524.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.