

Phosphonic acid, chloromethyl-, bis(p-tolyl) ester

Inchi:	InChI=1S/C15H16ClO3P/c1-12-3-7-14(8-4-12)18-20(17,11-16)19-15-9-5-13(2)6-10-15/h
InchiKey:	HRCCBPVNYXGUII-UHFFFAOYSA-N
Formula:	C15H16ClO3P
SMILES:	<chem>Cc1ccc(OP(=O)(CCl)Oc2ccc(C)cc2)cc1</chem>
Mol. weight [g/mol]:	310.71
CAS:	23896-95-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.82		Crippen Method
logp	5.151		Crippen Method
mcvol	225.000	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=C23896959&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

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