

2-Chlorophenyl bis(3-methylphenyl) phosphate

Inchi:	InChI=1S/C20H18ClO4P/c1-15-7-5-9-17(13-15)23-26(22,24-18-10-6-8-16(2)14-18)25-20
InchiKey:	DSNMVIMYFBEWMM-UHFFFAOYSA-N
Formula:	C20H18ClO4P
SMILES:	<chem>Cc1cccc(OP(=O)(Oc2cccc(C)c2)Oc2ccccc2Cl)c1</chem>
Mol. weight [g/mol]:	388.78
CAS:	116402-09-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.77		Crippen Method
logp	6.602		Crippen Method
mcvol	277.560	ml/mol	McGowan Method

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=C116402096&Units=SI

Legend

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

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