

5-Isopropyl-2-methylphenyl bis(2-methylphenyl) phosphate

Inchi:	InChI=1S/C24H27O4P/c1-17(2)21-15-14-20(5)24(16-21)28-29(25,26-22-12-8-6-10-18(22
InchiKey:	VUOFDTVTHHYDMU-UHFFFAOYSA-N
Formula:	C24H27O4P
SMILES:	<chem>Cc1ccccc1OP(=O)(Oc1ccccc1C)Oc1cc(C(C)C)ccc1C</chem>
Mol. weight [g/mol]:	410.44
CAS:	116402-12-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.75		Crippen Method
logp	7.380		Crippen Method
mcvol	321.680	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=C116402121&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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