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: Cc1ccccc1OP(=O)(Oc1ccccc1C)Oc1cc(C(C)C)ccc1C

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402121&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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