

Bis(5-isopropyl-2-methylphenyl) 2-methylphenyl phosphate

Inchi: InChI=1S/C27H33O4P/c1-18(2)23-14-12-21(6)26(16-23)30-32(28,29-25-11-9-8-10-20(25
InchiKey: KOQWSFRLEOTRFW-UHFFFAOYSA-N
Formula: C27H33O4P
SMILES: Cc1ccccc1OP(=O)(Oc1cc(C(C)C)ccc1C)Oc1cc(C(C)C)ccc1C
Mol. weight [g/mol]: 452.52
CAS: 116402-06-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.93		Crippen Method
logp	8.504		Crippen Method
mcvol	363.950	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402063&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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