

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(22-19-23-20))31-30-27-32-33-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100
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

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