4-Tert-butylphenyl bis(2-methylphenyl) phosphate

Inchi: InChI=1S/C24H27O4P/c1-18-10-6-8-12-22(18)27-29(25,28-23-13-9-7-11-19(23)2)26-21-

InchiKey: UTVBYAZNJDVVSV-UHFFFAOYSA-N

Formula: C24H27O4P

SMILES: Cc1ccccc1OP(=O)(Oc1ccc(C(C)(C)C)cc1)Oc1ccccc1C

Mol. weight [g/mol]: 410.44

CAS: 116402-07-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.40		Crippen Method
logp	7.246		Crippen Method
mcvol	321.680	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402074&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume