

Tris(2-cyclohexylphenyl) phosphate

Inchi: InChI=1S/C36H45O4P/c37-41(38-34-25-13-10-22-31(34)28-16-4-1-5-17-28,39-35-26-14
InchiKey: MKOXSOFBQGEZNV-UHFFFAOYSA-N
Formula: C36H45O4P
SMILES: O=P(Oc1ccccc1C1CCCCC1)(Oc1ccccc1C1CCCCC1)Oc1ccccc1C1CCCCC1
Mol. weight [g/mol]: 572.71
CAS: 116402-17-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.14		Crippen Method
logp	11.475		Crippen Method
mcvol	458.180	ml/mol	McGowan Method

Sources

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=C116402176&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

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<https://www.chemeo.com/cid/76-361-7/Tris-2-cyclohexylphenyl-phosphate.pdf>

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