

Tris(2,4-di-tert-butylphenyl) phosphate

Inchi: InChI=1S/C42H63O4P/c1-37(2,3)28-19-22-34(31(25-28)40(10,11)12)44-47(43,45-35-23-36)41-42
InchiKey: AZSKHRTUXHLAHS-UHFFFAOYSA-N
Formula: C42H63O4P
SMILES: CC(C)(C)c1ccc(OP(=O)(Oc2ccc(C(C)(C)C)cc2C(C)(C)C)Oc2ccc(C(C)(C)C)cc2C(C)(C)C)cc1
Mol. weight [g/mol]: 662.92
CAS: 95906-11-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-15.02		Crippen Method
logp	13.116		Crippen Method
mcvol	575.300	ml/mol	McGowan Method
rinpol	3582.30		NIST Webbook
rinpol	3582.30		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C95906119&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/123-273-2/Tris-2-4-di-tert-butylphenyl-phosphate.pdf>

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