

# Tris[4-(1,1,3,3-tetramethylbutyl)phenyl]phosphate

<b>Inchi:</b>	InChI=1S/C42H63O4P/c1-37(2,3)28-40(10,11)31-16-22-34(23-17-31)44-47(43,45-35-24
<b>InchiKey:</b>	OOMSKJURDQBDAO-UHFFFAOYSA-N
<b>Formula:</b>	C42H63O4P
<b>SMILES:</b>	CC(C)(C)CC(C)(C)c1ccc(OP(=O)(Oc2ccc(C(C)(C)CC(C)(C)C)cc2)Oc2ccc(C(C)(C)CC(C)(C)C)cc2)Oc2ccc(C(C)(C)CC(C)(C)C)cc2
<b>Mol. weight [g/mol]:</b>	662.92
<b>CAS:</b>	222552-35-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-15.38		Crippen Method
logp	13.473		Crippen Method
mcvol	575.300	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C222552354&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C222552354&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

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

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