

# Tris[4-(1-phenylethyl)phenyl] phosphate

<b>Inchi:</b>	InChI=1S/C42H39O4P/c1-31(34-13-7-4-8-14-34)37-19-25-40(26-20-37)44-47(43,45-41-2
<b>InchiKey:</b>	LVNYEUXPFPQSNE-UHFFFAOYSA-N
<b>Formula:</b>	C42H39O4P
<b>SMILES:</b>	CC(c1ccccc1)c1ccc(OP(=O)(Oc2ccc(C(C)c3ccccc3)cc2)Oc2ccc(C(C)c3ccccc3)cc2)cc1
<b>Mol. weight [g/mol]:</b>	638.73
<b>CAS:</b>	16960-08-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-14.59		Crippen Method
logp	11.787		Crippen Method
mcvol	504.020	ml/mol	McGowan Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C16960080&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16960080&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>

## 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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<https://www.chemeo.com/cid/74-604-9/Tris-4-1-phenylethyl-phenyl-phosphate.pdf>

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