

# 1-Naphthalenol, phosphate (3:1)

<b>Other names:</b>	1-Naphthol, phosphate (3:1) Phosphoric acid, tri-1-naphthyl ester
<b>Inchi:</b>	InChI=1S/C30H21O4P/c31-35(32-28-19-7-13-22-10-1-4-16-25(22)28,33-29-20-8-14-23-1
<b>InchiKey:</b>	DBPYGJOORSXBMI-UHFFFAOYSA-N
<b>Formula:</b>	C30H21O4P
<b>SMILES:</b>	O=P(Oc1cccc2ccccc12)(Oc1cccc2ccccc12)Oc1cccc2ccccc12
<b>Mol. weight [g/mol]:</b>	476.46
<b>CAS:</b>	4004-51-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-12.55		Crippen Method
logp	8.791		Crippen Method
mvol	347.840	ml/mol	McGowan Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4004517&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4004517&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

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

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