1-Naphthalenol, phosphate (3:1)

Other names:	1-Naphthol, phosphate (3:1)
	Phosphoric acid, tri-1-naphthyl ester
Inchi:	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
InchiKey:	DBPYGJOORSXBMI-UHFFFAOYSA-N
Formula:	C30H21O4P
SMILES:	O=P(Oc1cccc2ccccc12)(Oc1cccc2ccccc12)Oc1cccc2ccccc12
Mol. weight [g/mol]:	476.46
CAS:	4004-51-7

Physical Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4004517&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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