

Mono-octyl phosphate

Other names:	octyl dihydrogen phosphate
Inchi:	InChI=1S/C8H19O4P/c1-2-3-4-5-6-7-8-12-13(9,10)11/h2-8H2,1H3,(H2,9,10,11)
InchiKey:	WRKCIHRWQZQBOL-UHFFFAOYSA-N
Formula:	C8H19O4P
SMILES:	CCCCCCCCOP(=O)(O)O
Mol. weight [g/mol]:	210.21
CAS:	3991-73-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.05		Crippen Method
logp	2.456		Crippen Method
mcvol	167.520	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3991739&Units=SI
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

Legend

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

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