

Phosphoric acid, octadecyl ester

Other names:	octadecyl dihydrogen phosphate
Inchi:	InChI=1S/C18H39O4P/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-23(19,20)21/h
InchiKey:	UHGIMQLJWRAPLT-UHFFFAOYSA-N
Formula:	C18H39O4P
SMILES:	CCCCCCCCCCCCCCCCCOP(=O)(O)O
Mol. weight [g/mol]:	350.47
CAS:	2958-09-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.24		Crippen Method
logp	6.357		Crippen Method
mcvol	308.420	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2958090&Units=SI

Legend

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

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