

Diethyl dodecyl phosphate

Inchi:	InChI=1S/C16H35O4P/c1-4-7-8-9-10-11-12-13-14-15-16-20-21(17,18-5-2)19-6-3/h4-16H
InchiKey:	YBSWYHAWMOPART-UHFFFAOYSA-N
Formula:	C16H35O4P
SMILES:	CCCCCCCCCCCCOP(=O)(OCC)OCC
Mol. weight [g/mol]:	322.42
CAS:	91776-68-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.05		Crippen Method
logp	6.105		Crippen Method
mcvol	280.240	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91776680&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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