

Phosphoric acid, diethyl 2-ethylhexyl ester

Inchi:	InChI=1S/C12H27O4P/c1-5-9-10-12(6-2)11-16-17(13,14-7-3)15-8-4/h12H,5-11H2,1-4H3
InchiKey:	KSBHGUFVHFCKX-UHFFFAOYSA-N
Formula:	C12H27O4P
SMILES:	CCCCC(CC)COP(=O)(OCC)OCC
Mol. weight [g/mol]:	266.31
CAS:	88795-49-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.13		Crippen Method
logp	4.401		Crippen Method
mcvol	223.880	ml/mol	McGowan Method

Sources

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=C88795497&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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