

Dibutyl hydrogen phosphate

Inchi:	InChI=1S/C8H19O4P/c1-3-5-7-11-13(9,10)12-8-6-4-2/h3-8H2,1-2H3,(H,9,10)
InchiKey:	JYFHYPJRHGVZDY-UHFFFAOYSA-N
Formula:	C8H19O4P
SMILES:	CCCCOP(=O)(O)OCCCC
Mol. weight [g/mol]:	210.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.09		Aqueous Solubility Prediction Method
logp	2.720		Crippen Method
mcvol	167.520	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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