

Diethyl (4-biphenylmethyl)phosphonate

Inchi:	InChI=1S/C17H21O3P/c1-3-19-21(18,20-4-2)14-15-10-12-17(13-11-15)16-8-6-5-7-9-16/h
InchiKey:	HWKCLILHNFQFV-UHFFFAOYSA-N
Formula:	C17H21O3P
SMILES:	CCOP(=O)(Cc1ccc(-c2ccccc2)cc1)OCC
Mol. weight [g/mol]:	304.32
CAS:	30818-70-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.08		Crippen Method
logp	5.120		Crippen Method
mcvol	240.940	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=C30818703&Units=SI
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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<https://www.chemeo.com/cid/21-500-2/Diethyl-4-biphenylmethyl-phosphonate.pdf>

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