

Phosphonic acid, (phenylmethyl)-, diethyl ester

Other names:	Diethyl benzylphosphonate Benzylphosphonic acid diethyl ester Diethoxyphosphonomethylbenzene Diethyl phosphonate, benzyl- Phosphonic acid, benzyl-, diethyl ester
Inchi:	InChI=1S/C11H17O3P/c1-3-13-15(12,14-4-2)10-11-8-6-5-7-9-11/h5-9H,3-4,10H2,1-2H3
InchiKey:	AIPRAPZUGUTQKX-UHFFFAOYSA-N
Formula:	C11H17O3P
SMILES:	CCOP(=O)(Cc1ccccc1)OCC
Mol. weight [g/mol]:	228.22
CAS:	1080-32-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.47		Crippen Method
logp	3.453		Crippen Method
mcvol	180.160	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	441.00 ± 1.00	K	3.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1080326&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tbrp:	Boiling point at reduced pressure

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