

Phosphonic acid, (phenylmethyl)-, dimethyl ester

Other names:	Benzylphosphonic acid, dimethyl ester Dimethyl benzylphosphonate Phosphonic acid, benzyl-, dimethyl ester
Inchi:	InChI=1S/C9H13O3P/c1-11-13(10,12-2)8-9-6-4-3-5-7-9/h3-7H,8H2,1-2H3
InchiKey:	QLNYTKJCHFEIDA-UHFFFAOYSA-N
Formula:	C9H13O3P
SMILES:	COP(=O)(Cc1ccccc1)OC
Mol. weight [g/mol]:	200.17
CAS:	773-47-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.64		Crippen Method
logp	2.672		Crippen Method
mcvol	151.980	ml/mol	McGowan Method
rinsol	1530.00		NIST Webbook

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=C773477&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
rinsol:	Non-polar retention indices

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