

Phosphonic acid, phenyl-, diethyl ester

Other names:	Diethyl benzenephosphonate Diethyl phenylphosphonate Benzenephosphonic acid, diethyl ester Phenylphosphonic acid diethyl ester
Inchi:	InChI=1S/C10H15O3P/c1-3-12-14(11,13-4-2)10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3
InchiKey:	VZEGPPPCKHRYGO-UHFFFAOYSA-N
Formula:	C10H15O3P
SMILES:	CCOP(=O)(OCC)c1ccccc1
Mol. weight [g/mol]:	214.20
CAS:	1754-49-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.95		Crippen Method
logp	2.578		Crippen Method
mcvol	166.070	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1754490&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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