

Methyl diethylphosphonoacetate

Other names:	Diethylmethylphosphonoacetate Diethyl carbomethoxymethylphosphonate Acetic acid, (diethoxyphosphinyl)-, methyl ester Acetic acid, phosphono-, p,p-diethyl c-methyl ester
Inchi:	InChI=1S/C7H15O5P/c1-4-11-13(9,12-5-2)6-7(8)10-3/h4-6H2,1-3H3
InchiKey:	CTSAXXHOGZNKJR-UHFFFAOYSA-N
Formula:	C7H15O5P
SMILES:	CCOP(=O)(CC(=O)OC)OCC
Mol. weight [g/mol]:	210.16
CAS:	1067-74-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.06		Crippen Method
logp	1.425		Crippen Method
mcvol	155.000	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1067749&Units=SI

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/53-965-2/Methyl-diethylphosphonoacetate.pdf>

Generated by Cheméo on 2024-04-23 16:32:18.616503961 +0000 UTC m=+16179187.537081276.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.