

Methylphosphonic acid, methyl-(2-pentyl) ester

Other names:	Methylphosphonic acid, 2-pentyl, methyl ester
Inchi:	InChI=1S/C7H17O3P/c1-5-6-7(2)10-11(4,8)9-3/h7H,5-6H2,1-4H3
InchiKey:	OCPXKGSWJHMFWM-UHFFFAOYSA-N
Formula:	C7H17O3P
SMILES:	CCCC(C)OP(C)(=O)OC
Mol. weight [g/mol]:	180.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	2.661		Crippen Method
mcvol	147.560	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=R548459&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.chemeo.com/cid/98-643-0/Methylphosphonic-acid-methyl-2-pentyl-ester.pdf>

Generated by Cheméo on 2024-04-26 21:11:34.842469283 +0000 UTC m=+16455143.763046595.

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