

Methylphosphonic acid, methyl-(4-methyl-2-pentyl) ester

Inchi:	InChI=1S/C8H19O3P/c1-7(2)6-8(3)11-12(5,9)10-4/h7-8H,6H2,1-5H3
InchiKey:	UUWSXHSBLUIENO-UHFFFAOYSA-N
Formula:	C8H19O3P
SMILES:	COP(C)(=O)OC(C)CC(C)C
Mol. weight [g/mol]:	194.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	2.907		Crippen Method
mcvol	161.650	ml/mol	McGowan Method
rinpole	755.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R548479&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
rinpole:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/36-245-0/Methylphosphonic-acid-methyl-4-methyl-2-pentyl-ester.pdf>

Generated by Cheméo on 2024-04-26 14:52:03.740555742 +0000 UTC m=+16432372.661133060.

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