

Methyl methylphosphonofluoridate

Other names:	Phosphonofluoridic acid, methyl-, methyl ester Methylphosphonic acid, fluoroanhydride, methyl ester
Inchi:	InChI=1S/C2H6FO2P/c1-5-6(2,3)4/h1-2H3
InchiKey:	LEOIIUMNVNRPNW-UHFFFAOYSA-N
Formula:	C2H6FO2P
SMILES:	COP(C)(=O)F
Mol. weight [g/mol]:	112.04
CAS:	353-88-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.87		Crippen Method
logp	1.425		Crippen Method
mcvol	73.010	ml/mol	McGowan Method
rinpol	587.00		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	586.60		NIST Webbook
rinpol	586.60		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=C353888&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

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

rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/81-235-1/Methyl-methylphosphonofluoridate.pdf>

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