

Ethyl methylphosphonofluoridate

Other names:	Phosphonofluoric acid, methyl-, ethyl ester Methylphosphonic acid, fluoroanhydride-, ethyl ester Phosphonofluoric acid, P-methyl-, ethyl ester O-Ethyl methylphosphonofluoridate
Inchi:	InChI=1S/C3H8FO2P/c1-3-6-7(2,4)5/h3H2,1-2H3
InchiKey:	RIYPSXBGLXRZNJ-UHFFFAOYSA-N
Formula:	C3H8FO2P
SMILES:	CCOP(C)(=O)F
Mol. weight [g/mol]:	126.07
CAS:	673-97-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.29		Crippen Method
logp	1.815		Crippen Method
mcpvol	87.100	ml/mol	McGowan Method
rinpol	755.00		NIST Webbook
rinpol	754.90		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	754.90		NIST Webbook

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=C673972&Units=SI

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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