

Ethyl ethylphosphonofluoridate

Other names:	Phosphonofluoridic acid, ethyl-, ethyl ester
Inchi:	InChI=1S/C4H10FO2P/c1-3-7-8(5,6)4-2/h3-4H2,1-2H3
InchiKey:	RORQVZRCLFKMMP-UHFFFAOYSA-N
Formula:	C4H10FO2P
SMILES:	CCOP(=O)(F)CC
Mol. weight [g/mol]:	140.09
CAS:	650-20-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.71		Crippen Method
logp	2.205		Crippen Method
mcvol	101.190	ml/mol	McGowan Method
rinpol	866.00		NIST Webbook
rinpol	865.70		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	865.70		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=C650204&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/124-588-2/Ethyl-ethylphosphonofluoridate.pdf>

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