

Phosphonofluoridic acid, ethyl-, isopropyl ester

Other names:	Ethylphosphonofluoridic acid isopropyl ester Isopropoxy-ethylphosphonofluoridate Isopropoxy-ethyl-phosphoryl fluoride Phoshonofluoridic acid, ethyl-, isopropyl ester Ethylphoshonic acid, fluoroanhydride-, isopropyl ester Isopropyl ethylphosphonofluoridate
Inchi:	InChI=1S/C5H12FO2P/c1-4-9(6,7)8-5(2)3/h5H,4H2,1-3H3
InchiKey:	KXKAXOZWSFAJTG-UHFFFAOYSA-N
Formula:	C5H12FO2P
SMILES:	CCP(=O)(F)OC(C)C
Mol. weight [g/mol]:	154.12
CAS:	1189-87-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Crippen Method
logp	2.594		Crippen Method
mcvol	115.280	ml/mol	McGowan Method
rinpol	907.00		NIST Webbook
rinpol	906.90		NIST Webbook
rinpol	907.00		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=C1189873&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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