

Methyl ethylphosphonofluoridate

Other names: Phoshonofluoridic acid, ethyl-, methyl ester
Ethylphoshonic acid, fluoroanhydride-, methyl ester

Inchi: InChI=1S/C3H8FO2P/c1-3-7(4,5)6-2/h3H2,1-2H3

InchiKey: ZDJWQJGNAPPOHA-UHFFFAOYSA-N

Formula: C3H8FO2P

SMILES: CCP(=O)(F)OC

Mol. weight [g/mol]: 126.07

CAS: 665-03-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.29		Crippen Method
logp	1.815		Crippen Method
mcvol	87.100	ml/mol	McGowan Method
rinpol	803.00		NIST Webbook
rinpol	802.70		NIST Webbook
rinpol	803.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C665032&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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