Pentyl ethylphosphonofluoridate

Other names: Ethylphoshonic acid, fluoroanhydride, penthyl ester
Inchi: InChI=1S/C7H16FO2P/c1-3-5-6-7-10-11(8,9)4-2/h3-7H2,1-2H3
InchiKey: GYEBPDIEIHZFGM-UHFFFAOYSA-N
Formula: C7H16FO2P
SMILES: CCCCCOP(=O)(F)CC
Mol. weight [g/mol]: 182.17
CAS: 162085-84-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.97		Crippen Method
logp	3.376		Crippen Method
mcvol	143.460	ml/mol	McGowan Method
rinpol	1165.00		NIST Webbook
rinpol	1165.20		NIST Webbook
rinpol	1165.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C162085849&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