Phenyl methylphosphonofluoridate

Inchi: InChI=1S/C7H8FO2P/c1-11(8,9)10-7-5-3-2-4-6-7/h2-6H,1H3
InchiKey: UTQIOSIJOGSEHL-UHFFFAOYSA-N
Formula: C7H8FO2P
SMILES: CP(=O)(F)Oc1ccccc1
Mol. weight [g/mol]: 174.11
CAS: 133826-40-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.72		Crippen Method
logp	2.858		Crippen Method
mcvol	119.700	ml/mol	McGowan Method
rinpol	1207.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1207.00		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=C133826401&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from: