

Phosphonofluoridic acid, ethyl-, cyclopentyl ester

Other names:	Cyclopentyl ethylphosphonofluoridate Cyclopentyl ethylphosphonofluoridate
Inchi:	InChI=1S/C7H14FO2P/c1-2-11(8,9)10-7-5-3-4-6-7/h7H,2-6H2,1H3
InchiKey:	BMYQDWCAODOERJ-UHFFFAOYSA-N
Formula:	C7H14FO2P
SMILES:	CCP(=O)(F)OC1CCCC1
Mol. weight [g/mol]:	180.16
CAS:	345239-06-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.97		Crippen Method
logp	3.128		Crippen Method
mcvol	132.600	ml/mol	McGowan Method
rinpol	1199.00		NIST Webbook
rinpol	1199.00		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=C345239067&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

Latest version available from:

<https://www.cheméo.com/cid/122-780-0/Phosphonofluoridic-acid-ethyl-cyclopentyl-ester.pdf>

Generated by Cheméo on 2024-04-30 00:40:35.277395057 +0000 UTC m=+16726884.197972373.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.