

Phosphonofluoridic acid, methyl-, cycloheptyl ester

Other names:	Methylphosphonic acid, fluoroanhydride, cycloheptyl ester Cycloheptyl methylphosphonofluoridoate Cycloheptyl methylphosphonofluoridate
Inchi:	InChI=1S/C8H16FO2P/c1-12(9,10)11-8-6-4-2-3-5-7-8/h8H,2-7H2,1H3
InchiKey:	FLEZPAFIBXHSRI-UHFFFAOYSA-N
Formula:	C8H16FO2P
SMILES:	CP(=O)(F)OC1CCCCC1
Mol. weight [g/mol]:	194.18
CAS:	7284-83-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	3.518		Crippen Method
mcvol	146.690	ml/mol	McGowan Method
rinpol	1340.00		NIST Webbook
rinpol	1340.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7284835&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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