

cycloheptyl propylphosphonofluoridoate

Other names:	Cycloheptyl propylphosphonofluoridate
Inchi:	InChI=1S/C10H20FO2P/c1-2-9-14(11,12)13-10-7-5-3-4-6-8-10/h10H,2-9H2,1H3
InchiKey:	QQPJTW HNYFSLKY-UHFFFAOYSA-N
Formula:	C10H20FO2P
SMILES:	CCCP(=O)(F)OC1CCCCC1
Mol. weight [g/mol]:	222.24

Physical Properties

Property code	Value	Unit	Source
logp	4.298		Crippen Method
mcvol	174.870	ml/mol	McGowan Method
rinpol	1528.00		NIST Webbook
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Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U298297&Units=SI>

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/115-965-3/cycloheptyl-propylphosphonofluoridoate.pdf>

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