

Cycloheptyl ethylphosphonofluoridoate

Other names: Cycloheptyl ethylphosphonofluoridate
Inchi: InChI=1S/C9H18FO2P/c1-2-13(10,11)12-9-7-5-3-4-6-8-9/h9H,2-8H2,1H3
InchiKey: MRBLOSDYQOWWOZ-UHFFFAOYSA-N
Formula: C9H18FO2P
SMILES: CCP(=O)(F)OC1CCCCC1
Mol. weight [g/mol]: 208.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.81		Crippen Method
logp	3.908		Crippen Method
mcvol	160.780	ml/mol	McGowan Method
rinpola	1438.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U298448&Units=SI>
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>

Legend

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

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<https://www.chemeo.com/cid/119-403-2/Cycloheptyl-ethylphosphonofluoridoate.pdf>

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