

Cyclobutyl ethylphosphonofluoridoate

Other names: Cyclobutyl ethylphosphonofluoridate
Inchi: InChI=1S/C6H12FO2P/c1-2-10(7,8)9-6-4-3-5-6/h6H,2-5H2,1H3
InchiKey: OZSZZVZOWFTUMI-UHFFFAOYSA-N
Formula: C6H12FO2P
SMILES: CCP(=O)(F)OC1CCC1
Mol. weight [g/mol]: 166.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	2.738		Crippen Method
mcvol	118.510	ml/mol	McGowan Method
rinpol	1098.00		NIST Webbook
rinpol	1098.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U298327&Units=SI>

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.chemeo.com/cid/77-788-3/Cyclobutyl-ethylphosphonofluoridoate.pdf>

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