

Cyclohexyl methylphosphonothionofluoridate

Inchi: InChI=1S/C7H14FOPS/c1-10(8,11)9-7-5-3-2-4-6-7/h7H,2-6H2,1H3
InchiKey: PZXWAMVRPZGTDV-UHFFFAOYSA-N
Formula: C7H14FOPS
SMILES: CP(F)(=S)OC1CCCCC1
Mol. weight [g/mol]: 196.22
CAS: 4241-34-3

Physical Properties

Property code	Value	Unit	Source
log10ws	1.04		Crippen Method
logp	3.244		Crippen Method
mcvol	143.080	ml/mol	McGowan Method
rinpol	1250.00		NIST Webbook
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rinpol	1250.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4241343&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

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