

Hexyl ethylphosphonofluoridate

Inchi: InChI=1S/C8H18FO2P/c1-3-5-6-7-8-11-12(9,10)4-2/h3-8H2,1-2H3
InchiKey: ZYXRWBNFAGZKON-UHFFFAOYSA-N
Formula: C8H18FO2P
SMILES: CCCCCCOP(=O)(F)CC
Mol. weight [g/mol]: 196.20
CAS: 135445-19-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	3.766		Crippen Method
mcvol	157.550	ml/mol	McGowan Method
rinpol	1265.00		NIST Webbook
rinpol	1265.30		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1265.30		NIST Webbook

Sources

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=C135445191&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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