

Heptyl ethylphosphonofluoridate

Other names:	Ethylphosphonic acid, fluoroanhydride, heptyl ester
Inchi:	InChI=1S/C9H20FO2P/c1-3-5-6-7-8-9-12-13(10,11)4-2/h3-9H2,1-2H3
InchiKey:	CQXIORRIIAXLOU-UHFFFAOYSA-N
Formula:	C9H20FO2P
SMILES:	CCCCCCCOP(=O)(F)CC
Mol. weight [g/mol]:	210.23
CAS:	162085-85-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.80		Crippen Method
logp	4.156		Crippen Method
mcvol	171.640	ml/mol	McGowan Method
rinpol	1364.00		NIST Webbook
rinpol	1364.20		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1364.00		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=C162085850&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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