

n-Heptyl methylphosphonofluoridate

Other names:	Methylphosphonic acid, fluoroanhydride, heptyl ester Heptyl methylphosphonofluoridate Phosphonofluoridic acid, P-methyl-, heptyl ester Phosphonofluoridic acid, methyl-, heptyl ester
Inchi:	InChI=1S/C8H18FO2P/c1-3-4-5-6-7-8-11-12(2,9)10/h3-8H2,1-2H3
InchiKey:	CVKLOBCYWQJDHP-UHFFFAOYSA-N
Formula:	C8H18FO2P
SMILES:	CCCCCCCOP(C)(=O)F
Mol. weight [g/mol]:	196.20
CAS:	162085-82-7

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	1272.40		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1272.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C162085827&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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