

Ethyl isopropyl dimethylphosphoramidate

Other names:	Ethyl isopropyl N,N-dimethylphosphoramidate
Inchi:	InChI=1S/C7H18NO3P/c1-6-10-12(9,8(4)5)11-7(2)3/h7H,6H2,1-5H3
InchiKey:	VWONBITUNATGHP-UHFFFAOYSA-N
Formula:	C7H18NO3P
SMILES:	CCOP(=O)(OC(C)C)N(C)C
Mol. weight [g/mol]:	195.20
CAS:	99520-56-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.87		Crippen Method
logp	2.118		Crippen Method
mcvol	157.540	ml/mol	McGowan Method
rinpol	1121.00		NIST Webbook
rinpol	1166.60		NIST Webbook
rinpol	1121.40		NIST Webbook
rinpol	1166.60		NIST Webbook
rinpol	1121.40		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=C99520566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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