

Diethyl-5-hydantolylylphosphonate

Inchi:	InChI=1S/C7H13N2O5P/c1-3-14-15(12,4-13-2)6-5(10)8-7(11)9-6/h6H,3-4H2,1-2H3,(H2,8)
InchiKey:	GKFZWWSTGPKIM-UHFFFAOYSA-N
Formula:	C7H13N2O5P
SMILES:	CCOP(=O)(COC)C1NC(=O)NC1=O
Mol. weight [g/mol]:	236.16
CAS:	95378-36-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	0.070		Crippen Method
mcvol	159.800	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95378362&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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