

Phosdrin,«beta»

Inchi:	InChI=1S/C7H13O6P/c1-6(5-7(8)10-2)13-14(9,11-3)12-4/h5H,1-4H3
InchiKey:	GEPDYQSQVLXLEU-UHFFFAOYSA-N
Formula:	C7H13O6P
SMILES:	<chem>COC(=O)C=C(C)OP(=O)(OC)OC</chem>
Mol. weight [g/mol]:	224.15

Physical Properties

Property code	Value	Unit	Source
hvap	70.51	kJ/mol	Cheméo Relay (1.0)
log10ws	-0.06		Cheméo Relay (1.0)
logp	1.481		Crippen Method
mcvol	156.570	ml/mol	McGowan Method
rinpol	1390.00		NIST Webbook
rinpol	1446.00		NIST Webbook
tb	533.04	K	Cheméo Relay (1.0)
tf	271.47	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R296445&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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