Phosdrin, «alpha»

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: COC(=O)C=C(C)OP(=O)(OC)OC
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	1392.00		NIST Webbook
rinpol	1446.00		NIST Webbook
tb	533.04	K	Cheméo Relay (1.0)
tf	271.47	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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=R296430&Units=SI

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