Diethylhydroxymethyl phosphonate

Other names:	(Hydroxymethyl)phosphonic acid, diethyl ester
	Phosphonic acid, (hydroxymethyl)-, diethyl ester
Inchi:	InChI=1S/C5H13O4P/c1-3-8-10(7,5-6)9-4-2/h6H,3-5H2,1-2H3
InchiKey:	RWIGWWBLTJLKMK-UHFFFAOYSA-N
Formula:	C5H13O4P
SMILES:	CCOP(=O)(CO)OCC
Mol. weight [g/mol]:	168.13

Physical Properties

Property code	Value	Unit	Source
hvap	71.35	kJ/mol	Cheméo Relay (1.0)
ie	10.29	eV	Cheméo Relay (1.0)
log10ws	0.42		Cheméo Relay (1.0)
logp	1.202		Crippen Method
mcvol	125.250	ml/mol	McGowan Method
tb	515.94	K	Cheméo Relay (1.0)
tf	246.33	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3084400&Units=SI
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

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point