Methylphosphonic acid, 3-methyl-1-butyl, methyl ester

Other names: Methylphosphonic acid, 3-methyl-1-butyl, methyl ester
Inchi: InChI=1S/C7H17O3P/c1-7(2)5-6-10-11(4,8)9-3/h7H,5-6H2,1-4H3
InchiKey: QCVGEMUTTZNUGZ-UHFFFAOYSA-N
Formula: C7H17O3P
SMILES: COP(C)(=O)OCCC(C)C
Mol. weight [g/mol]: 180.18

Physical Properties

Property code	Value	Unit	Source
hvap	61.02	kJ/mol	Cheméo Relay (1.0)
ie	9.84	eV	Cheméo Relay (1.0)
logp	2.518		Crippen Method
mcvol	147.560	ml/mol	McGowan Method
rinpol	697.00		NIST Webbook
rinpol	697.00		NIST Webbook
rinpol	697.00		NIST Webbook
tb	498.37	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=R548464&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

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature