Methyl-phosphonic acid pinacolyl ester methyl ester, diastereomer 1

Other names: Methyl-phosphonic acid pinacolyl ester methyl ester, diastereomer 1
Inchi: InChI=1S/C8H19O3P/c1-7(8(2,3)4)11-12(6,9)10-5/h7H,1-6H3
InchiKey: IVTOWMZAZSBKOT-UHFFFAOYSA-N
Formula: C8H19O3P
SMILES: COP(C)(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 194.21

Physical Properties

Property code	Value	Unit	Source
hvap	60.74	kJ/mol	Cheméo Relay (1.0)
ie	9.60	eV	Cheméo Relay (1.0)
logp	2.907		Crippen Method
mcvol	161.650	ml/mol	McGowan Method
rinpol	1200.00		NIST Webbook
rinpol	1200.00		NIST Webbook
tb	494.14	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=R266518&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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