Triethyl-4-phosphonocrotonate

Other names: Triethyl 4-phosphonocrotonate
2-Butenoic acid, 2-(diethoxyphosphinyl)-, ethyl ester
ethyl 2-(diethoxyphosphinyl)but-2-enoate
Inchi: InChI=1S/C10H19O5P/c1-4-13-10(11)8-7-9-16(12,14-5-2)15-6-3/h7-8H,4-6,9H2,1-3H3/b
InchiKey: LXLODBXSCRTXFG-BQYQJAHWSA-N
Formula: C10H19O5P
SMILES: CCOC(=O)/C=C/CP(=O)(OCC)OCC
Mol. weight [g/mol]: 250.23

Physical Properties

Property code	Value	Unit	Source
af	0.6141		Cheméo Relay (1.0)
hf	-961.84	kJ/mol	Cheméo Relay (1.0)
hvap	77.08	kJ/mol	Cheméo Relay (1.0)
ie	9.68	eV	Cheméo Relay (1.0)
log10ws	-1.44		Cheméo Relay (1.0)
logp	2.372		Crippen Method
mcvol	192.970	ml/mol	McGowan Method
pc	2037.47	kPa	Cheméo Relay (1.0, beta)
tb	575.79	K	Cheméo Relay (1.0)
tc	715.08	K	Cheméo Relay (1.0)
tf	238.69	K	Cheméo Relay (1.0)
vc	0.703	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20345624&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

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume