

Triethyl «gamma»-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=CCP(=O)(OCC)OCC
Mol. weight [g/mol]:	250.23
CAS:	20345-62-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	2.372		Crippen Method
mcvol	192.970	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20345624&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/76-763-1/Triethyl-gamma-phosphonocrotonate.pdf>

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