

Triethyl 4-phosphonobutanoate

Other names:	Triethyl-4-phosphono butyrate Butanoic acid, 4-(diethoxyphosphinyl)-, ethyl ester Butyric acid, 4-diethylphosphono-, ethyl ester
Inchi:	InChI=1S/C10H21O5P/c1-4-13-10(11)8-7-9-16(12,14-5-2)15-6-3/h4-9H2,1-3H3
InchiKey:	FYESTJSRASJZOY-UHFFFAOYSA-N
Formula:	C10H21O5P
SMILES:	CCOC(=O)CCCP(=O)(OCC)OCC
Mol. weight [g/mol]:	252.24
CAS:	2327-69-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.32		Crippen Method
logp	2.596		Crippen Method
mcvol	197.270	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=C2327697&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/90-993-0/Triethyl-4-phosphonobutanoate.pdf>

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