

Butonate

Inchi:	InChI=1S/C8H14Cl3O5P/c1-4-5-6(12)16-7(8(9,10)11)17(13,14-2)15-3/h7H,4-5H2,1-3H3
InchiKey:	BKAQXYNWONVOAX-UHFFFAOYSA-N
Formula:	C8H14Cl3O5P
SMILES:	CCCC(=O)OC(C(Cl)(Cl)Cl)P(=O)(OC)OC
Mol. weight [g/mol]:	327.53
CAS:	126-22-7

Physical Properties

Property code	Value	Unit	Source
ie	10.30	eV	NIST Webbook
log10ws	-4.65		Crippen Method
logp	3.512		Crippen Method
mcvol	205.810	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C126227&Units=SI

Legend

ie:	Ionization energy
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/33-884-4/Butonate.pdf>

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