

Phosphinic acid, bis(chloromethyl),- ethyl ester

Other names:	Ethyl bis[chloromethyl]phosphinate
Inchi:	InChI=1S/C4H9Cl2O2P/c1-2-8-9(7,3-5)4-6/h2-4H2,1H3
InchiKey:	ZOQQHTTYHSLXKY-UHFFFAOYSA-N
Formula:	C4H9Cl2O2P
SMILES:	CCOP(=O)(CCl)CCl
Mol. weight [g/mol]:	190.99
CAS:	13274-84-5

Physical Properties

Property code	Value	Unit	Source
ie	10.19	eV	NIST Webbook
log10ws	-3.16		Crippen Method
logp	2.694		Crippen Method
mcvol	123.900	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=C13274845&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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