

Phosphoryl chloride fluoride

Inchi:	InChI=1S/Cl2FOP/c1-5(2,3)4
InchiKey:	YNECJZSONMVFHE-UHFFFAOYSA-N
Formula:	Cl2FOP
SMILES:	O=P(F)(Cl)Cl
Mol. weight [g/mol]:	136.88
CAS:	13769-76-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	2.542		Crippen Method
mcvol	63.440	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13769761&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/38-165-7/Phosphoryl-chloride-fluoride.pdf>

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