

Phosgard 2xc20

Other names:	2,2-bis(chloromethyl)trimethylene bis(bis(2-chloroethyl)phosphate)
Inchi:	InChI=1S/C13H24Cl6O8P2/c14-1-5-22-28(20,23-6-2-15)26-11-13(9-18,10-19)12-27-29(2
InchiKey:	ZGHUDSLVQAGWEY-UHFFFAOYSA-N
Formula:	C13H24Cl6O8P2
SMILES:	O=P(OCCCI)(OCCCI)OCC(CCI)(CCI)COP(=O)(OCCCI)OCCCI
Mol. weight [g/mol]:	582.99
CAS:	38051-10-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.99		Crippen Method
logp	5.721		Crippen Method
mcvol	355.350	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=C38051104&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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