

Phosgard c-22r (monsanto)

Other names:	1-[bis(2-chloroethoxyphosphinyl)ethyl 2-chloroethyl
Inchi:	[1-[[[2-chloroethoxy)(2-chloroethyl)phosphinyl]oxy]ethyl]phosphonate InChI=1S/C14H28Cl5O9P3/c1-13(27-29(20,12-7-19)23-8-3-15)31(22,26-11-6-18)28-14(2
InchiKey:	QDLQFWNOQPOPHV-UHFFFAOYSA-N
Formula:	C14H28Cl5O9P3
SMILES:	CC(OP(=O)(OCCCI)C(C)OP(=O)(CCCI)OCCCI)P(=O)(OCCCI)OCCCI
Mol. weight [g/mol]:	610.55
CAS:	4351-70-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.01		Crippen Method
logp	6.551		Crippen Method
mcvol	383.530	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=C4351706&Units=SI

Legend

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

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