

# Phosgard b52r (monsanto)

<b>Inchi:</b>	InChI=1S/C14H24Br4Cl4O6P2/c1-10(28-30(24,14(2-15)6-22)27-9-13(18)5-21)29(23,25-
<b>InchiKey:</b>	KINBREMVZFOQIJ-UHFFFAOYSA-N
<b>Formula:</b>	C14H24Br4Cl4O6P2
<b>SMILES:</b>	CC(OP(=O)(OCC(Br)CCI)C(CCl)CBr)P(=O)(OCC(Br)CCI)OCC(Br)CCI
<b>Mol. weight [g/mol]:</b>	811.71
<b>CAS:</b>	25079-53-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.97		Crippen Method
logp	7.794		Crippen Method
mcvol	403.220	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C25079532&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C25079532&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

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

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