

2-Propanol, 1,3-dibromo-, phosphate (3:1)

Other names:	Tris(1,3-dibromo-2-propyl)phosphate Tris(1-bromomethyl-2-bromoethyl)phosphate
Inchi:	InChI=1S/C9H15Br6O4P/c10-1-7(2-11)17-20(16,18-8(3-12)4-13)19-9(5-14)6-15/h7-9H,1
InchiKey:	RZEYUZWXPABTCN-UHFFFAOYSA-N
Formula:	C9H15Br6O4P
SMILES:	O=P(OC(CBr)CBr)(OC(CBr)CBr)OC(CBr)CBr
Mol. weight [g/mol]:	697.61
CAS:	18713-51-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.04		Crippen Method
logp	5.620		Crippen Method
mcvol	286.610	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=C18713514&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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