

Bis(2-bromoethyl) 2-bromoethylphosphonate

Inchi: InChI=1S/C6H12Br3O3P/c7-1-4-11-13(10,6-3-9)12-5-2-8/h1-6H2
InchiKey: KKGVBGGAVZGMKA-UHFFFAOYSA-N
Formula: C6H12Br3O3P
SMILES: O=P(CCBBr)(OCCBr)OCCBr
Mol. weight [g/mol]: 402.84
CAS: 78-45-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	3.397		Crippen Method
mcvol	185.970	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=C78455&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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