

Diethyl 3-bromophenyl phosphate

Inchi: InChI=1S/C10H14BrO4P/c1-3-13-16(12,14-4-2)15-10-7-5-6-9(11)8-10/h5-8H,3-4H2,1-2H
InchiKey: RJWJYUAVFOHPSK-UHFFFAOYSA-N
Formula: C10H14BrO4P
SMILES: CCOP(=O)(OCC)Oc1cccc(Br)c1
Mol. weight [g/mol]: 309.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.45		Crippen Method
logp	4.009		Crippen Method
mcvol	189.440	ml/mol	McGowan Method
rinpole	1777.00		NIST Webbook
rinpole	1777.00		NIST Webbook
ripole	2490.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R168924&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices
ripole: Polar retention indices

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