

Dimethyl 4-bromophenyl phosphate

Inchi: InChI=1S/C8H10BrO4P/c1-11-14(10,12-2)13-8-5-3-7(9)4-6-8/h3-6H,1-2H3
InchiKey: QEQBXPUBBUQQSW-UHFFFAOYSA-N
Formula: C8H10BrO4P
SMILES: COP(=O)(OC)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 281.04

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	3.229		Crippen Method
mcvol	161.260	ml/mol	McGowan Method
rinpol	1666.00		NIST Webbook
rinpol	1666.00		NIST Webbook
ripol	2410.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R169016&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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