

Dimethyl 3-bromophenyl phosphate

Inchi: InChI=1S/C8H10BrO4P/c1-11-14(10,12-2)13-8-5-3-4-7(9)6-8/h3-6H,1-2H3
InchiKey: JVTOXSUYRIBMHP-UHFFFAOYSA-N
Formula: C8H10BrO4P
SMILES: COP(=O)(OC)Oc1cccc(Br)c1
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	1652.00		NIST Webbook
ripol	2392.00		NIST Webbook

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=R168964&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
rinpol: Non-polar retention indices
ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/40-220-2/Dimethyl-3-bromophenyl-phosphate.pdf>

Generated by Cheméo on 2024-04-30 08:04:26.724060569 +0000 UTC m=+16753515.644637884.
Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.