

3-Bromobenzoic acid, morpholide

Inchi: InChI=1S/C11H12BrNO2/c12-10-3-1-2-9(8-10)11(14)13-4-6-15-7-5-13/h1-3,8H,4-7H2
InchiKey: ZVHMYYPYPSUJGLHH-UHFFFAOYSA-N
Formula: C11H12BrNO2
SMILES: O=C(c1cccc(Br)c1)N1CCOCC1
Mol. weight [g/mol]: 270.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.60		Crippen Method
logp	1.922		Crippen Method
mcvol	166.150	ml/mol	McGowan Method
rinpole	1921.00		NIST Webbook
rinpole	1921.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307150&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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