2-Bromobenzoic acid, morpholide

Inchi: InChI=1S/C11H12BrNO2/c12-10-4-2-1-3-9(10)11(14)13-5-7-15-8-6-13/h1-4H,5-8H2
InchiKey: QPQCGIYRAMNHKH-UHFFFAOYSA-N
Formula: C11H12BrNO2
SMILES: O=C(c1ccccc1Br)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
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307382&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.