

2-Chlorobenzoic acid, morpholide

Inchi: InChI=1S/C11H12ClNO2/c12-10-4-2-1-3-9(10)11(14)13-5-7-15-8-6-13/h1-4H,5-8H2
InchiKey: ZRGHSGNYLSCFJY-UHFFFAOYSA-N
Formula: C11H12ClNO2
SMILES: O=C(c1ccccc1Cl)N1CCOCC1
Mol. weight [g/mol]: 225.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	1.812		Crippen Method
mcvol	160.890	ml/mol	McGowan Method
rinpole	1799.00		NIST Webbook
rinpole	1799.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U306976&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpole: Non-polar retention indices

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<https://www.chemeo.com/cid/118-679-8/2-Chlorobenzoic-acid-morpholide.pdf>

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