

3-Chloropropionic acid, morpholide

Inchi: InChI=1S/C7H12ClNO2/c8-2-1-7(10)9-3-5-11-6-4-9/h1-6H2
InchiKey: RHPBOUGBOGWTDW-UHFFFAOYSA-N
Formula: C7H12ClNO2
SMILES: O=C(CCCl)N1CCOCC1
Mol. weight [g/mol]: 177.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.23		Crippen Method
logp	0.474		Crippen Method
mcvol	128.290	ml/mol	McGowan Method
rinsol	1440.00		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=U307223&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

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<https://www.chemeo.com/cid/13-176-2/3-Chloropropionic-acid-morpholide.pdf>

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