

Cyclobutanecarboxylic acid, morpholide

Inchi: InChI=1S/C9H15NO2/c11-9(8-2-1-3-8)10-4-6-12-7-5-10/h8H,1-7H2
InchiKey: PNAUTTGUBWLOMQ-UHFFFAOYSA-N
Formula: C9H15NO2
SMILES: O=C(C1CCC1)N1CCOCC1
Mol. weight [g/mol]: 169.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.57		Crippen Method
logp	0.645		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
rinpol	1459.00		NIST Webbook
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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=U307044&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

Latest version available from:

<https://www.chemeo.com/cid/35-173-1/Cyclobutanecarboxylic-acid-morpholide.pdf>

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