

Cyclopropanecarboxylic acid, morpholide

Inchi: InChI=1S/C8H13NO2/c10-8(7-1-2-7)9-3-5-11-6-4-9/h7H,1-6H2
InchiKey: UXMTWEKYJARZAK-UHFFFAOYSA-N
Formula: C8H13NO2
SMILES: O=C(C1CC1)N1CCOCC1
Mol. weight [g/mol]: 155.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.15		Crippen Method
logp	0.255		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
rinpol	1352.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307183&Units=SI>

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/36-112-7/Cyclopropanecarboxylic-acid-morpholide.pdf>

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