

Cyclopentanecarboxylic acid, morpholide

Inchi: InChI=1S/C10H17NO2/c12-10(9-3-1-2-4-9)11-5-7-13-8-6-11/h9H,1-8H2
InchiKey: ANSZQSWDZKSRTA-UHFFFAOYSA-N
Formula: C10H17NO2
SMILES: O=C(C1CCCC1)N1CCOCC1
Mol. weight [g/mol]: 183.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.99		Crippen Method
logp	1.035		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
rinpol	1556.00		NIST Webbook
rinpol	1556.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=U307022&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/85-729-9/Cyclopentanecarboxylic-acid-morpholide.pdf>

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