

Pentanoic acid, morpholide

Inchi: InChI=1S/C9H17NO2/c1-2-3-4-9(11)10-5-7-12-8-6-10/h2-8H2,1H3
InchiKey: AASPBTJOWALDEO-UHFFFAOYSA-N
Formula: C9H17NO2
SMILES: CCCCC(=O)N1CCOCC1
Mol. weight [g/mol]: 171.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.92		Crippen Method
logp	1.035		Crippen Method
mcvol	144.230	ml/mol	McGowan Method
rinpol	1403.00		NIST Webbook
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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=U306888&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/62-268-6/Pentanoic-acid-morpholide.pdf>

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