

2-Methylpropionic acid, morpholide

Inchi: InChI=1S/C8H15NO2/c1-7(2)8(10)9-3-5-11-6-4-9/h7H,3-6H2,1-2H3
InchiKey: GSBBRQAUAKEVIN-UHFFFAOYSA-N
Formula: C8H15NO2
SMILES: CC(C)C(=O)N1CCOCC1
Mol. weight [g/mol]: 157.21

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -0.26 | | Crippen Method |
| logp | 0.501 | | Crippen Method |
| mcvol | 130.140 | ml/mol | McGowan Method |
| rinpol | 1256.00 | | NIST Webbook |
| rinpol | 1256.00 | | 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=U307317&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/57-834-3/2-Methylpropionic-acid-morpholide.pdf>

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