

Acetoxyacetic acid, morpholide

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|-----------------------------|---|
| Inchi: | InChI=1S/C8H13NO4/c1-7(10)13-6-8(11)9-2-4-12-5-3-9/h2-6H2,1H3 |
| InchiKey: | ZOEMPWSIKOJFAH-UHFFFAOYSA-N |
| Formula: | C8H13NO4 |
| SMILES: | CC(=O)OCC(=O)N1CCOCC1 |
| Mol. weight [g/mol]: | 187.19 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | 0.64 | | Crippen Method |
| logp | -0.592 | | Crippen Method |
| mcvol | 137.580 | ml/mol | McGowan Method |
| rinpola | 1490.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U307088&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| rinpola: | Non-polar retention indices |

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<https://www.chemeo.com/cid/44-540-3/Acetoxyacetic-acid-morpholide.pdf>

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