

Methoxyacetic acid, morpholide

Inchi: InChI=1S/C7H13NO3/c1-10-6-7(9)8-2-4-11-5-3-8/h2-6H2,1H3
InchiKey: GGMGHASWIYSLRL-UHFFFAOYSA-N
Formula: C7H13NO3
SMILES: COCC(=O)N1CCOCC1
Mol. weight [g/mol]: 159.18

Physical Properties

Property code	Value	Unit	Source
log10ws	0.83		Crippen Method
logp	-0.508		Crippen Method
mcvol	121.920	ml/mol	McGowan Method
rinpole	1282.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307254&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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
rinpole: Non-polar retention indices

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<https://www.chemeo.com/cid/37-107-2/Methoxyacetic-acid-morpholide.pdf>

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