

3-Methyl-2-butenic acid, morpholide

Inchi: InChI=1S/C9H15NO2/c1-8(2)7-9(11)10-3-5-12-6-4-10/h7H,3-6H2,1-2H3
InchiKey: LWMJXIONGBCNT-UHFFFAOYSA-N
Formula: C9H15NO2
SMILES: CC(C)=CC(=O)N1CCOCC1
Mol. weight [g/mol]: 169.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.77		Crippen Method
logp	0.811		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
rinpol	1396.00		NIST Webbook
rinpol	1396.00		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=U307265&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

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<https://www.chemeo.com/cid/19-183-8/3-Methyl-2-butenic-acid-morpholide.pdf>

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