2,2-Dimethylpropionic acid, morpholide

Inchi: InChI=1S/C9H17NO2/c1-9(2,3)8(11)10-4-6-12-7-5-10/h4-7H2,1-3H3
InchiKey: ZNYMSOJUAJANBK-UHFFFAOYSA-N
Formula: C9H17NO2
SMILES: CC(C)(C)C(=O)N1CCOCC1
Mol. weight [g/mol]: 171.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.68		Crippen Method
logp	0.891		Crippen Method
mcvol	144.230	ml/mol	McGowan Method
rinpol	1305.00		NIST Webbook
rinpol	1305.00		NIST Webbook

Sources

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=U307192&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.