

3-Phenylpropionic acid, morpholide

Inchi: InChI=1S/C13H17NO2/c15-13(14-8-10-16-11-9-14)7-6-12-4-2-1-3-5-12/h1-5H,6-11H2
InchiKey: UYUYDGNUIQSIJW-UHFFFAOYSA-N
Formula: C13H17NO2
SMILES: O=C(CCc1cccc1)N1CCOCC1
Mol. weight [g/mol]: 219.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.69		Crippen Method
logp	1.478		Crippen Method
mcvol	176.830	ml/mol	McGowan Method
rinpol	1887.00		NIST Webbook
rinpol	1887.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308112&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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