

Cyclo-Ile-Pro-diketopiperazine

Inchi: InChI=1S/C11H18N2O2/c1-3-7(2)9-11(15)13-6-4-5-8(13)10(14)12-9/h7-9H,3-6H2,1-2H3
InchiKey: ZDACRNZBFJOLTC-UHFFFAOYSA-N
Formula: C11H18N2O2
SMILES: CCC(C)C1NC(=O)C2CCCN2C1=O
Mol. weight [g/mol]: 210.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.51		Crippen Method
logp	0.522		Crippen Method
mcvol	167.230	ml/mol	McGowan Method
rinpol	1478.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R225473&Units=SI>
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>

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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