

Cyclo-Ala-Pro-diketopiperazine

Inchi: InChI=1S/C8H12N2O2/c1-5-8(12)10-4-2-3-6(10)7(11)9-5/h5-6H,2-4H2,1H3,(H,9,11)
InchiKey: WSLYCILIEOFQPK-UHFFFAOYSA-N
Formula: C8H12N2O2
SMILES: CC1NC(=O)C2CCCN2C1=O
Mol. weight [g/mol]: 168.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.49		Crippen Method
logp	-0.504		Crippen Method
mcvol	124.960	ml/mol	McGowan Method
rinpol	1259.00		NIST Webbook
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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=R225468&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

Latest version available from:

<https://www.chemeo.com/cid/61-678-2/Cyclo-Ala-Pro-diketopiperazine.pdf>

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