Cyclo-Val-Pro-diketopiperazine

Inchi: InChI=1S/C10H16N2O2/c1-6(2)8-10(14)12-5-3-4-7(12)9(13)11-8/h6-8H,3-5H2,1-2H3,(H,
InchiKey: XLUAWXQORJEMBD-UHFFFAOYSA-N
Formula: C10H16N2O2
SMILES: CC(C)C1NC(=O)C2CCCN2C1=O
Mol. weight [g/mol]: 196.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.09		Crippen Method
logp	0.132		Crippen Method
mcvol	153.140	ml/mol	McGowan Method
rinpol	1376.00		NIST Webbook
rinpol	1376.00		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=R225522&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

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