

I-Proline, N-caproyl-, methyl ester

Inchi: InChI=1S/C12H21NO3/c1-3-4-5-8-11(14)13-9-6-7-10(13)12(15)16-2/h10H,3-9H2,1-2H3
InchiKey: UJMPCCUZXBILS-UHFFFAOYSA-N
Formula: C12H21NO3
SMILES: CCCCCC(=O)N1CCCC1C(=O)OC
Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.06		Crippen Method
logp	1.731		Crippen Method
mcvol	188.070	ml/mol	McGowan Method
rinpol	1721.00		NIST Webbook
rinpol	1721.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299735&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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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