

I-Proline, N-butyryl-, methyl ester

Inchi: InChI=1S/C10H17NO3/c1-3-5-9(12)11-7-4-6-8(11)10(13)14-2/h8H,3-7H2,1-2H3
InchiKey: YDOXTIOAUXVDHL-UHFFFAOYSA-N
Formula: C10H17NO3
SMILES: CCCC(=O)N1CCCC1C(=O)OC
Mol. weight [g/mol]: 199.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.22		Crippen Method
logp	0.951		Crippen Method
mcvol	159.890	ml/mol	McGowan Method
rinpol	1530.00		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=U308816&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

Latest version available from:

<https://www.chemeo.com/cid/60-587-4/l-Proline-N-butyryl-methyl-ester.pdf>

Generated by Cheméo on 2024-04-19 19:27:23.68453598 +0000 UTC m=+15844092.605113296.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.