L-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: UJMPCCUZXBIYLS-UHFFFAOYSA-N
Formula: C12H21NO3
SMILES: CCCCCC(=O)N1CCCC1C(=O)OC
Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.51		Cheméo Relay (1.0)
logp	1.731		Crippen Method
mcvol	188.070	ml/mol	McGowan Method
rinpol	1721.00		NIST Webbook
rinpol	1721.00		NIST Webbook
tf	315.16	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299735&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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
tf: Normal melting (fusion) point