L-Pro, N-ethoxycarbonyl, (S)-1-phenylethylamide

Inchi: InChI=1S/C16H22N2O3/c1-3-21-16(20)18-11-7-10-14(18)15(19)17-12(2)13-8-5-4-6-9-13

InchiKey: FCMOKSLYERJIEZ-GXTWGEPZSA-N

Formula: C16H22N2O3

SMILES: CCOC(=O)N1CCCC1C(=O)NC(C)c1ccccc1

Mol. weight [g/mol]: 290.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	2.485		Crippen Method
mcvol	230.650	ml/mol	McGowan Method
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R587647&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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