D-Pipecolic acid, N-ethoxycarbonyl, (S)-1-phenylethylamide

Inchi: InChI=1S/C17H24N2O3/c1-3-22-17(21)19-12-8-7-11-15(19)16(20)18-13(2)14-9-5-4-6-10

InchiKey: ZIMZRTQSTJRFHY-DZGCQCFKSA-N

Formula: C17H24N2O3

SMILES: CCOC(=O)N1CCCCC1C(=O)NC(C)c1ccccc1

Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.88		Crippen Method
logp	2.875		Crippen Method
mcvol	244.740	ml/mol	McGowan Method
rinpol	2214.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R587518&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices