D-Pipecolic acid, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi: InChI=1S/C14H25NO4/c1-5-18-14(17)15-9-7-6-8-12(15)13(16)19-11(4)10(2)3/h10-12H,5

InchiKey: VFRHGYSFWMKXKS-PXYINDEMSA-N

Formula: C14H25NO4

SMILES: CCOC(=O)N1CCCCC1C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 271.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Crippen Method
logp	2.585		Crippen Method
mcvol	222.120	ml/mol	McGowan Method
rinpol	1750.60		NIST Webbook
rinpol	1750.60		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=R501930&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

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