Pipecolylpipecolic acid, N-propoxycarbonyl-, propyl ester

Inchi: InChI=1S/C19H32N2O5/c1-3-13-25-18(23)16-10-6-7-11-20(16)17(22)15-9-5-8-12-21(15)19(24)26-14-4-2

InchiKey: SWBZDPDQDHLOSX-UHFFFAOYSA-N

Formula: C19H32N2O5

SMILES: CCCOC(=O)C1CCCCN1C(=O)C1CCCCN1C(=O)OCCC

Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	2.722		Crippen Method
mcvol	293.260	ml/mol	McGowan Method
rinpol	2547.00		NIST Webbook
rinpol	2547.00		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=U393009&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

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