Pipecolylpipecolylpipecolic acid, N-ethoxycarbonyl-, ethyl ester

Inchi: InChI=1S/C23H37N3O6/c1-3-31-22(29)19-13-7-9-15-25(19)20(27)17-11-5-8-14-24(17)21

InchiKey: YCHSEONDDSZZSN-UHFFFAOYSA-N

Formula: C23H37N3O6

SMILES: CCOC(=O)C1CCCCN1C(=O)C1CCCCN1C(=O)C1CCCCN1C(=O)OCC

Mol. weight [g/mol]: 451.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	2.323		Crippen Method
mcvol	350.310	ml/mol	McGowan Method
rinpol	3234.00		NIST Webbook
rinpol	3234.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393092&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.