Pipecolylpipecolic acid, N-ethoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C22H38N2O5/c1-3-5-6-7-12-17-29-21(26)19-14-9-10-15-23(19)20(25)18-13-8-

InchiKey: PMVGGHMKJVNVFE-UHFFFAOYSA-N

Formula: C22H38N2O5

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

Mol. weight [g/mol]: 410.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.66		Crippen Method
logp	3.892		Crippen Method
mcvol	335.530	ml/mol	McGowan Method
rinpol	2876.00		NIST Webbook
rinpol	2876.00		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=U393085&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

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