Pipecolic acid, N-propoxycarbonyl-, octyl ester

Inchi: InChI=1S/C18H33NO4/c1-3-5-6-7-8-11-15-22-17(20)16-12-9-10-13-19(16)18(21)23-14-4

InchiKey: LUNGQBLSUAULLO-UHFFFAOYSA-N

Formula: C18H33NO4

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

Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	4.291		Crippen Method
mcvol	278.480	ml/mol	McGowan Method
rinpol	2269.00		NIST Webbook
rinpol	2269.00		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=U392999&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.