Pipecolic acid, N-propoxycarbonyl-, pentyl ester

Inchi: InChI=1S/C15H27NO4/c1-3-5-8-12-19-14(17)13-9-6-7-10-16(13)15(18)20-11-4-2/h13H,3

InchiKey: ZVZZQEBSHUGJSD-UHFFFAOYSA-N

Formula: C15H27NO4

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

Mol. weight [g/mol]: 285.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.38		Crippen Method
logp	3.121		Crippen Method
mcvol	236.210	ml/mol	McGowan Method
rinpol	1974.00		NIST Webbook
rinpol	1974.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392996&Units=SI

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

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.