Pipecolic acid, N-octyloxycarbonyl-, pentyl ester

Inchi: InChI=1S/C20H37NO4/c1-3-5-7-8-9-13-17-25-20(23)21-15-11-10-14-18(21)19(22)24-16-

InchiKey: PEZOQAXCGZXSGH-UHFFFAOYSA-N

Formula: C20H37NO4

SMILES: CCCCCCCCOC(=O)N1CCCCC1C(=O)OCCCCC

Mol. weight [g/mol]: 355.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.47		Crippen Method
logp	5.071		Crippen Method
mcvol	306.660	ml/mol	McGowan Method
rinpol	2438.00		NIST Webbook
rinpol	2438.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393126&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.