Pipecolic acid, N-octyloxycarbonyl-, heptyl ester

Inchi: InChI=1S/C22H41NO4/c1-3-5-7-9-11-15-19-27-22(25)23-17-13-12-16-20(23)21(24)26-18

InchiKey: GADLLBHFIKEAOF-UHFFFAOYSA-N

Formula: C22H41NO4

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

Mol. weight [g/mol]: 383.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.31		Crippen Method
logp	5.852		Crippen Method
mcvol	334.840	ml/mol	McGowan Method
rinpol	2640.00		NIST Webbook
rinpol	2640.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393128&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.