Pipecolic acid, N-octyloxycarbonyl-, hexyl ester

Inchi: InChI=1S/C21H39NO4/c1-3-5-7-9-10-14-18-26-21(24)22-16-12-11-15-19(22)20(23)25-17

InchiKey: ORQOTBLGSQXNHL-UHFFFAOYSA-N

Formula: C21H39NO4

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

Mol. weight [g/mol]: 369.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.89		Crippen Method
logp	5.462		Crippen Method
mcvol	320.750	ml/mol	McGowan Method
rinpol	2539.00		NIST Webbook
rinpol	2539.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393127&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.