Pipecolic acid, N-propoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C17H31NO4/c1-3-5-6-7-10-14-21-16(19)15-11-8-9-12-18(15)17(20)22-13-4-2/h
InchiKey: GHUMQKJUBFCMHU-UHFFFAOYSA-N
Formula: C17H31NO4
SMILES: CCCCCCCOC(=O)C1CCCCN1C(=O)OCCC
Mol. weight [g/mol]: 313.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.22		Crippen Method
logp	3.901		Crippen Method
mcvol	264.390	ml/mol	McGowan Method
rinpol	2168.00		NIST Webbook
rinpol	2168.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392998&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.