Pipecolic acid, N-butoxycarbonyl-, pentyl ester

Inchi: InChI=1S/C16H29NO4/c1-3-5-9-13-20-15(18)14-10-7-8-11-17(14)16(19)21-12-6-4-2/h14
InchiKey: AQJFVOIVYXIBJZ-UHFFFAOYSA-N
Formula: C16H29NO4
SMILES: CCCCCOC(=O)C1CCCCN1C(=O)OCCCC
Mol. weight [g/mol]: 299.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	3.511		Crippen Method
mcvol	250.300	ml/mol	McGowan Method
rinpol	2042.00		NIST Webbook
rinpol	2042.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393051&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.