L-Proline, N-octanoyl-, butyl ester

Inchi: InChI=1S/C17H31NO3/c1-3-5-7-8-9-12-16(19)18-13-10-11-15(18)17(20)21-14-6-4-2/h15
InchiKey: UKNMACMEQYQFJL-UHFFFAOYSA-N
Formula: C17H31NO3
SMILES: CCCCCCCC(=O)N1CCCC1C(=O)OCCCC
Mol. weight [g/mol]: 297.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.15		Crippen Method
logp	3.681		Crippen Method
mcvol	258.520	ml/mol	McGowan Method
rinpol	2237.00		NIST Webbook
rinpol	2237.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346240&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.