Pipecolic acid, N-propargyloxycarbonyl-, undecyl ester

Inchi: InChI=1S/C21H35NO4/c1-3-5-6-7-8-9-10-11-14-18-25-20(23)19-15-12-13-16-22(19)21(2

InchiKey: PXVDDGPWIOURMC-UHFFFAOYSA-N

Formula: C21H35NO4

SMILES: C#CCOC(=O)N1CCCCC1C(=O)OCCCCCCCCCCC

Mol. weight [g/mol]: 365.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	4.685		Crippen Method
mcvol	312.150	ml/mol	McGowan Method
rinpol	2604.00		NIST Webbook
rinpol	2604.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393098&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.