Pipecolic acid, N-propargyloxycarbonyl-, tridecyl ester

Inchi: InChI=1S/C23H39NO4/c1-3-5-6-7-8-9-10-11-12-13-16-20-27-22(25)21-17-14-15-18-24(2

InchiKey: JLGFBJMKRZOBCY-UHFFFAOYSA-N

Formula: C23H39NO4

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

Mol. weight [g/mol]: 393.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.52		Crippen Method
logp	5.465		Crippen Method
mcvol	340.330	ml/mol	McGowan Method
rinpol	2807.00		NIST Webbook
rinpol	2807.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393100&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.