Pipecolylpipecolic acid, N-propargyloxycarbonyl-, heptyl ester

Inchi: InChI=1S/C23H36N2O5/c1-3-5-6-7-12-18-29-22(27)20-14-9-10-15-24(20)21(26)19-13-8-

InchiKey: XSCCQDBJNJVDNV-UHFFFAOYSA-N

Formula: C23H36N2O5

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

Mol. weight [g/mol]: 420.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.88		Crippen Method
logp	3.505		Crippen Method
mcvol	341.020	ml/mol	McGowan Method
rinpol	2952.00		NIST Webbook
rinpol	2952.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393105&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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