Pipecolic acid, N-propargyloxycarbonyl-, propargyl ester

Inchi: InChI=1S/C13H15NO4/c1-3-9-17-12(15)11-7-5-6-8-14(11)13(16)18-10-4-2/h1-2,11H,5-1

InchiKey: LTXXAOVXUBXRCL-UHFFFAOYSA-N

Formula: C13H15NO4

SMILES: C#CCOC(=O)C1CCCCN1C(=O)OCC#C

Mol. weight [g/mol]: 249.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	0.787		Crippen Method
mcvol	190.830	ml/mol	McGowan Method
rinpol	1808.00		NIST Webbook
rinpol	1808.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393101&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.