Pipecolylpipecolic acid, N-propargyloxycarbonyl-, nonyl ester

Inchi: InChI=1S/C25H40N2O5/c1-3-5-6-7-8-9-14-20-31-24(29)22-16-11-12-17-26(22)23(28)21-

InchiKey: JIBRCZCLCZHGNM-UHFFFAOYSA-N

Formula: C25H40N2O5

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

Mol. weight [g/mol]: 448.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.71		Crippen Method
logp	4.286		Crippen Method
mcvol	369.200	ml/mol	McGowan Method
rinpol	3150.00		NIST Webbook
rinpol	3150.00		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=U393107&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.