

Pipecolylpipecolic acid, N-propargyloxycarbonyl-, pentyl ester

Inchi: InChI=1S/C21H32N2O5/c1-3-5-10-16-27-20(25)18-12-7-8-13-22(18)19(24)17-11-6-9-14
InchiKey: VFPKOJKJIRVQJZ-UHFFFAOYSA-N
Formula: C21H32N2O5
SMILES: C#CCOC(=O)N1CCCCC1C(=O)N1CCCCC1C(=O)OCCCCC
Mol. weight [g/mol]: 392.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Crippen Method
logp	2.725		Crippen Method
mcvol	312.840	ml/mol	McGowan Method
rmpol	2766.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U393103&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rmpol: Non-polar retention indices

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