

Pipecolylpipecolic acid, N-propargyloxycarbonyl-, octyl ester

Inchi: InChI=1S/C24H38N2O5/c1-3-5-6-7-8-13-19-30-23(28)21-15-10-11-16-25(21)22(27)20-14
InchiKey: BHTMIQVYPPKHLZ-UHFFFAOYSA-N
Formula: C24H38N2O5
SMILES: C#CCOC(=O)N1CCCCC1C(=O)N1CCCCC1C(=O)OCCCCCCCC
Mol. weight [g/mol]: 434.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.29		Crippen Method
logp	3.896		Crippen Method
mcvol	355.110	ml/mol	McGowan Method
rinpol	3046.00		NIST Webbook
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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=U393106&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

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