Pipecolylpipecolic acid, N-propargyloxycarbonyl-, hexyl ester

Inchi: InChI=1S/C22H34N2O5/c1-3-5-6-11-17-28-21(26)19-13-8-9-14-23(19)20(25)18-12-7-10-
InchiKey: VCTWFEJBNNEBJA-UHFFFAOYSA-N
Formula: C22H34N2O5
SMILES: C#CCOC(=O)N1CCCCC1C(=O)N1CCCCC1C(=O)OCCCCCC
Mol. weight [g/mol]: 406.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.46		Crippen Method
logp	3.115		Crippen Method
mcvol	326.930	ml/mol	McGowan Method
rinpol	2857.00		NIST Webbook
rinpol	2857.00		NIST Webbook

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=U393104&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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