

Pipecolic acid, N-propargyloxycarbonyl-, pentyl ester

Inchi: InChI=1S/C15H23NO4/c1-3-5-8-12-19-14(17)13-9-6-7-10-16(13)15(18)20-11-4-2/h2,13H
InchiKey: UOCIWEIZTMZREM-UHFFFAOYSA-N
Formula: C15H23NO4
SMILES: C#CCOC(=O)N1CCCCC1C(=O)OCCCCC
Mol. weight [g/mol]: 281.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	2.344		Crippen Method
mcvol	227.610	ml/mol	McGowan Method
rinpol	1987.00		NIST Webbook
rinpol	1987.00		NIST Webbook

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=U393093&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

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