Pipecolic acid, N-propargyloxycarbonyl-, hexyl ester

Inchi: InChI=1S/C16H25NO4/c1-3-5-6-9-13-20-15(18)14-10-7-8-11-17(14)16(19)21-12-4-2/h2,1

InchiKey: HICHRLQMQQPDRA-UHFFFAOYSA-N

Formula: C16H25NO4

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

Mol. weight [g/mol]: 295.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.734		Crippen Method
mcvol	241.700	ml/mol	McGowan Method
rinpol	2085.00		NIST Webbook
rinpol	2085.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393094&Units=SI

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

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.