1-Aminocyclopentanecarboxylic acid, N-(propargyloxycarbonyl)-, pentyl ester

Inchi: InChI=1S/C15H23NO4/c1-3-5-8-12-19-13(17)15(9-6-7-10-15)16-14(18)20-11-4-2/h2H,3,5

InchiKey: UDMYYIWPEPBBLM-UHFFFAOYSA-N

Formula: C15H23NO4

SMILES: C#CCOC(O)=NC1(C(=O)OCCCCC)CCCC1

Mol. weight [g/mol]: 281.35

Physical Properties

Property code	Value	Unit	Source
hf	-442.13	kJ/mol	Joback Method
hvap	79.59	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.596		Crippen Method
mcvol	227.610	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1949.00		NIST Webbook
tb	815.69	K	Joback Method
tc	1023.95	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392465&Units=SI

Legend

hf: Enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature