1-Aminocyclopentanecarboxylic acid, N-(but-3-yn-1-yloxycarbonyl)-, decyl ester

Inchi: InChI=1S/C21H35NO4/c1-3-5-7-8-9-10-11-14-18-25-19(23)21(15-12-13-16-21)22-20(24)

InchiKey: GHAGDFNYBOJABL-UHFFFAOYSA-N

Formula: C21H35NO4

SMILES: C#CCCOC(O)=NC1(C(=O)OCCCCCCCCCC)CCCC1

Mol. weight [g/mol]: 365.51

Physical Properties

Property code	Value	Unit	Source
hf	-565.97	kJ/mol	Joback Method
hvap	92.94	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	4.937		Crippen Method
mcvol	312.150	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	2490.00		NIST Webbook
tb	952.97	K	Joback Method
tc	1167.88	K	Joback Method

Sources

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=U392573&Units=SI

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

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