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

Inchi: InChI=1S/C22H37NO4/c1-3-5-7-8-9-10-11-12-15-19-26-20(24)22(16-13-14-17-22)23-21(

InchiKey: XKDFGGLCIQHDTP-UHFFFAOYSA-N

Formula: C22H37NO4

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

Mol. weight [g/mol]: 379.53

Physical Properties

Property code	Value	Unit	Source
hf	-586.61	kJ/mol	Joback Method
hvap	95.17	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	5.327		Crippen Method
mcvol	326.240	ml/mol	McGowan Method
pc	1160.08	kPa	Joback Method
rinpol	2586.00		NIST Webbook
rinpol	2586.00		NIST Webbook
tb	975.85	K	Joback Method
tc	1194.85	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=U392574&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