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

Inchi: InChI=1S/C23H39NO4/c1-3-5-7-8-9-10-11-12-13-16-20-27-21(25)23(17-14-15-18-23)24-

InchiKey: VSYCIZBCLODWGL-UHFFFAOYSA-N

Formula: C23H39NO4

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

Mol. weight [g/mol]: 393.56

Physical Properties

Property code	Value	Unit	Source
hf	-607.25	kJ/mol	Joback Method
hvap	97.39	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	5.717		Crippen Method
mcvol	340.330	ml/mol	McGowan Method
pc	1087.78	kPa	Joback Method
tb	998.73	K	Joback Method
tc	1222.85	K	Joback Method

Sources

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=U392575&Units=SI

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

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature