1-Aminocyclopentanecarboxylic acid, N-(but-2-yn-1-yloxycarbonyl)-, octyl ester

Inchi: InChI=1S/C19H31NO4/c1-3-5-7-8-9-12-16-23-17(21)19(13-10-11-14-19)20-18(22)24-15-

InchiKey: IOIGYYGYLAWUNB-UHFFFAOYSA-N

Formula: C19H31NO4

SMILES: CC#CCOC(O)=NC1(C(=O)OCCCCCCCC)CCCC1

Mol. weight [g/mol]: 337.45

Physical Properties

Property code	Value	Unit	Source
hf	-544.29	kJ/mol	Joback Method
hvap	90.78	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.157		Crippen Method
mcvol	283.970	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
tb	926.09	K	Joback Method
tc	1141.04	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392582&Units=SI

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

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