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

Inchi: InChI=1S/C20H33NO4/c1-3-5-7-8-9-10-13-17-24-18(22)20(14-11-12-15-20)21-19(23)25-

InchiKey: WROHVWXTCBJJLC-UHFFFAOYSA-N

Formula: C20H33NO4

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

Mol. weight [g/mol]: 351.48

Physical Properties

Property code	Value	Unit	Source
hf	-564.93	kJ/mol	Joback Method
hvap	93.01	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.547		Crippen Method
mcvol	298.060	ml/mol	McGowan Method
pc	1339.80	kPa	Joback Method
rinpol	2484.00		NIST Webbook
rinpol	2484.00		NIST Webbook
tb	948.97	K	Joback Method
tc	1165.83	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392583&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

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