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

Inchi: InChI=1S/C25H43NO4/c1-3-5-7-8-9-10-11-12-13-14-15-18-22-29-23(27)25(19-16-17-20-

InchiKey: KSAJJRAIMLKSEV-UHFFFAOYSA-N

Formula: C25H43NO4

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

Mol. weight [g/mol]: 421.61

Physical Properties

Property code	Value	Unit	Source
hf	-668.13	kJ/mol	Joback Method
hvap	104.14	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	6.497		Crippen Method
mcvol	368.510	ml/mol	McGowan Method
pc	969.28	kPa	Joback Method
rinpol	2963.00		NIST Webbook
rinpol	2963.00		NIST Webbook
tb	1063.37	K	Joback Method
tc	1304.60	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392588&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