2-Aminopent-4-enoic acid, N-(but-2-yn-1-yloxycarbonyl)-, dodecyl ester

Inchi: InChI=1S/C22H37NO4/c1-4-7-9-10-11-12-13-14-15-16-19-26-21(24)20(17-6-3)23-22(25)

InchiKey: YPFZFDOQSDXBJQ-UHFFFAOYSA-N

Formula: C22H37NO4

SMILES: C=CCC(N=C(O)OCC#CC)C(=O)OCCCCCCCCCCCC

Mol. weight [g/mol]: 379.53

Physical Properties

Property code	Value	Unit	Source
hf	-561.78	kJ/mol	Joback Method
hvap	97.30	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.349		Crippen Method
mcvol	332.800	ml/mol	McGowan Method
pc	1041.25	kPa	Joback Method
rinpol	2664.00		NIST Webbook
rinpol	2664.00		NIST Webbook
tb	975.45	K	Joback Method
tc	1194.75	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393196&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