2-Aminopent-4-enoic acid, N-(but-3-en-1-yloxycarbonyl)-, undecyl ester

Inchi: InChI=1S/C21H37NO4/c1-4-7-9-10-11-12-13-14-15-18-25-20(23)19(16-6-3)22-21(24)26-

InchiKey: DVLOFAKOLGPTBQ-UHFFFAOYSA-N

Formula: C21H37NO4

SMILES: C=CCCOC(O)=NC(CC=C)C(=O)OCCCCCCCCCCC

Mol. weight [g/mol]: 367.52

Physical Properties

Property code	Value	Unit	Source
hf	-688.01	kJ/mol	Joback Method
hvap	92.25	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.512		Crippen Method
mcvol	323.010	ml/mol	McGowan Method
pc	1026.63	kPa	Joback Method
rinpol	2427.00		NIST Webbook
rinpol	2427.00		NIST Webbook
tb	940.25	K	Joback Method
tc	1152.01	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393208&Units=SI

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