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

Inchi: InChI=1S/C23H41NO4/c1-4-7-9-10-11-12-13-14-15-16-17-20-27-22(25)21(18-6-3)24-23(

InchiKey: OFUIBVPAZVALCF-UHFFFAOYSA-N

Formula: C23H41NO4

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

Mol. weight [g/mol]: 395.58

Physical Properties

Property code	Value	Unit	Source
hf	-729.29	kJ/mol	Joback Method
hvap	96.70	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	6.292		Crippen Method
mcvol	351.190	ml/mol	McGowan Method
pc	911.08	kPa	Joback Method
rinpol	2628.00		NIST Webbook
rinpol	2628.00		NIST Webbook
tb	986.01	K	Joback Method
tc	1213.01	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393205&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