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

Inchi: InChI=1S/C22H39NO4/c1-4-7-9-10-11-12-13-14-15-16-19-26-21(24)20(17-6-3)23-22(25)

InchiKey: AQGOWVKRQRCMMC-UHFFFAOYSA-N

Formula: C22H39NO4

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

Mol. weight [g/mol]: 381.55

Physical Properties

Property code	Value	Unit	Source
hf	-708.65	kJ/mol	Joback Method
hvap	94.48	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.902		Crippen Method
mcvol	337.100	ml/mol	McGowan Method
pc	966.27	kPa	Joback Method
rinpol	2532.00		NIST Webbook
rinpol	2532.00		NIST Webbook
tb	963.13	K	Joback Method
tc	1181.93	K	Joback Method

Sources

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=U393204&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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