

1-Aminocyclopentanecarboxylic acid, N-(but-3-en-1-yloxycarbonyl)-, undecyl ester

Inchi: InChI=1S/C22H39NO4/c1-3-5-7-8-9-10-11-12-15-19-26-20(24)22(16-13-14-17-22)23-21
InchiKey: SDHBIJUEMAYSAO-UHFFFAOYSA-N
Formula: C22H39NO4
SMILES: C=CCCOC(O)=NC1(C(=O)OCCCCCCCCCCCC)CCCC1
Mol. weight [g/mol]: 381.55

Physical Properties

Property code	Value	Unit	Source
hf	-753.08	kJ/mol	Joback Method
hvap	94.64	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.880		Crippen Method
mcpvol	330.540	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	2564.00		NIST Webbook
rinpol	2564.00		NIST Webbook
tb	982.41	K	Joback Method
tc	1202.88	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U392599&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
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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

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