

L-Norvaline, N-(but-3-en-1-yloxycarbonyl)-, undecyl ester

Inchi:	InChI=1S/C21H39NO4/c1-4-7-9-10-11-12-13-14-15-18-25-20(23)19(16-6-3)22-21(24)26
InchiKey:	ZUQLCUIQWGEWKG-LJQANCHMSA-N
Formula:	C21H39NO4
SMILES:	C=CCCOC(O)=NC(CCC)C(=O)OCCCCCCCCCCC
Mol. weight [g/mol]:	369.54

Physical Properties

Property code	Value	Unit	Source
hf	-813.44	kJ/mol	Joback Method
hvap	92.92	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.736		Crippen Method
mcvol	327.310	ml/mol	McGowan Method
pc	999.54	kPa	Joback Method
rinpol	2472.00		NIST Webbook
rinpol	2472.00		NIST Webbook
tb	943.57	K	Joback Method
tc	1156.81	K	Joback Method

Sources

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=U392873&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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