

L-Norvaline, N-(but-2-yn-1-yloxy carbonyl)-, octyl ester

Inchi:	InChI=1S/C18H31NO4/c1-4-7-9-10-11-12-15-22-17(20)16(13-6-3)19-18(21)23-14-8-5-2/
InchiKey:	GIPQQZAHAGIEQI-MRXNPFEDSA-N
Formula:	C18H31NO4
SMILES:	CC#CCOC(O)=NC(CCC)C(=O)OCCCCCCCC
Mol. weight [g/mol]:	325.44

Physical Properties

Property code	Value	Unit	Source
hf	-604.65	kJ/mol	Joback Method
hvap	89.06	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.013		Crippen Method
mcvol	280.740	ml/mol	McGowan Method
pc	1315.61	kPa	Joback Method
rinpol	2298.00		NIST Webbook
rinpol	2298.00		NIST Webbook
tb	887.25	K	Joback Method
tc	1089.30	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=U392865&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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