

L-Norvaline, N-(but-2-yn-1-yloxycarbonyl)-, pentyl ester

Inchi:	InChI=1S/C15H25NO4/c1-4-7-9-12-19-14(17)13(10-6-3)16-15(18)20-11-8-5-2/h13H,4,6-
InchiKey:	XLDHEEAOKFBTLT-CYBMUJFWSA-N
Formula:	C15H25NO4
SMILES:	CC#CCOC(O)=NC(CCC)C(=O)OCCCC
Mol. weight [g/mol]:	283.36

Physical Properties

Property code	Value	Unit	Source
hf	-542.73	kJ/mol	Joback Method
hvap	82.39	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.842		Crippen Method
mcvol	238.470	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	2013.00		NIST Webbook
rinpol	2013.00		NIST Webbook
tb	818.61	K	Joback Method
tc	1015.82	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U392862&Units=SI

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

Latest version available from:

<https://www.cheméo.com/cid/83-639-1/L-Norvaline-N-but-2-yn-1-yloxycarbonyl-pentyl-ester.pdf>

Generated by Cheméo on 2024-05-02 23:34:54.061833849 +0000 UTC m=+16982142.982411164.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.