

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

Inchi:	InChI=1S/C14H19NO4/c1-4-7-10-18-13(16)12(9-6-3)15-14(17)19-11-8-5-2/h12H,6,9-11H
InchiKey:	IYRVKEKPxDVZMZ-GFCCVEGCSA-N
Formula:	C14H19NO4
SMILES:	CC#CCOC(=O)NC(CCC)C(=O)OCC#CC
Mol. weight [g/mol]:	265.31

Physical Properties

Property code	Value	Unit	Source
gf	91.71	kJ/mol	Joback Method
hf	-229.10	kJ/mol	Joback Method
hfus	45.41	kJ/mol	Joback Method
hvap	75.42	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	1.471		Crippen Method
mvol	215.780	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	2001.00		NIST Webbook
rinpol	2001.00		NIST Webbook
tb	740.03	K	Joback Method
tc	953.20	K	Joback Method
tf	641.72	K	Joback Method
vc	0.821	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.07	J/mol×K	740.03	Joback Method
cpg	602.36	J/mol×K	775.56	Joback Method
cpg	615.75	J/mol×K	811.09	Joback Method
cpg	628.25	J/mol×K	846.61	Joback Method
cpg	639.84	J/mol×K	882.14	Joback Method
cpg	650.53	J/mol×K	917.67	Joback Method
cpg	660.31	J/mol×K	953.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392867&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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