

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

Inchi:

InChI=1S/C14H23NO4/c1-4-7-10-18-13(16)12(9-6-3)15-14(17)19-11-8-5-2/h12H,4,6-7,9

InchiKey:

SSUIVHMTPORNSJ-GFCCVEGCSA-N

Formula:

C14H23NO4

SMILES:

CC#CCOC(=O)NC(CCC)C(=O)OCCCC

Mol. weight [g/mol]:

269.34

Physical Properties

Property code	Value	Unit	Source
gf	-111.09	kJ/mol	Joback Method
hf	-501.40	kJ/mol	Joback Method
hfus	42.29	kJ/mol	Joback Method
hvap	73.27	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.248		Crippen Method
mcvol	224.380	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	1927.00		NIST Webbook
rinpol	1927.00		NIST Webbook
tb	731.03	K	Joback Method
tc	926.74	K	Joback Method
tf	535.62	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.23	J/mol×K	731.03	Joback Method
cpg	650.14	J/mol×K	763.65	Joback Method
cpg	664.19	J/mol×K	796.27	Joback Method
cpg	677.40	J/mol×K	828.89	Joback Method
cpg	689.76	J/mol×K	861.50	Joback Method
cpg	701.29	J/mol×K	894.12	Joback Method
cpg	711.98	J/mol×K	926.74	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=U392861&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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