

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

Inchi:	InChI=1S/C14H23NO4/c1-5-7-9-18-14(17)15-12(8-6-2)13(16)19-10-11(3)4/h11-12H,6,8-
InchiKey:	CYKIIULNSVDJFX-GFCCVEGCSA-N
Formula:	C14H23NO4
SMILES:	CC#CCOC(=O)NC(CCC)C(=O)OCC(C)C
Mol. weight [g/mol]:	269.34

Physical Properties

Property code	Value	Unit	Source
gf	-113.53	kJ/mol	Joback Method
hf	-506.68	kJ/mol	Joback Method
hfus	38.76	kJ/mol	Joback Method
hvap	72.88	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.104		Crippen Method
mcvol	224.380	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpola	1888.00		NIST Webbook
rinpola	1888.00		NIST Webbook
tb	730.59	K	Joback Method
tc	929.12	K	Joback Method
tf	520.62	K	Joback Method
vc	0.853	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.76	J/mol×K	730.59	Joback Method
cpg	650.90	J/mol×K	763.68	Joback Method
cpg	665.15	J/mol×K	796.77	Joback Method
cpg	678.52	J/mol×K	829.86	Joback Method
cpg	691.01	J/mol×K	862.95	Joback Method
cpg	702.63	J/mol×K	896.04	Joback Method
cpg	713.38	J/mol×K	929.12	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=U392860&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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