

L-Norvaline, N-isobutoxycarbonyl-, isobutyl ester

Inchi:	InChI=1S/C14H27NO4/c1-6-7-12(13(16)18-8-10(2)3)15-14(17)19-9-11(4)5/h10-12H,6-9H
InchiKey:	DORYDQPUROJTJO-UHFFFAOYSA-N
Formula:	C14H27NO4
SMILES:	CCCC(NC(=O)OCC(C)C)C(=O)OCC(C)C
Mol. weight [g/mol]:	273.37

Physical Properties

Property code	Value	Unit	Source
af	0.7889		Cheméo Relay (1.0)
hf	-987.69	kJ/mol	Cheméo Relay (1.0)
hfus	32.12	kJ/mol	Joback Method
hvap	78.62	kJ/mol	Cheméo Relay (1.0)
ie	9.03	eV	Cheméo Relay (1.0)
log10ws	-3.48		Cheméo Relay (1.0)
logp	2.736		Crippen Method
mcvol	232.980	ml/mol	McGowan Method
pc	1689.34	kPa	Joback Method
rinpol	1585.00		NIST Webbook
tb	559.14	K	Cheméo Relay (1.0)
tc	735.73	K	Cheméo Relay (1.0)
tf	282.26	K	Cheméo Relay (1.0)
vc	0.865	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.45	J/mol×K	721.15	Joback Method
cpg	698.41	J/mol×K	752.17	Joback Method
cpg	713.50	J/mol×K	783.18	Joback Method
cpg	727.73	J/mol×K	814.20	Joback Method
cpg	741.09	J/mol×K	845.22	Joback Method
cpg	753.60	J/mol×K	876.24	Joback Method
cpg	765.26	J/mol×K	907.25	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320714&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point
vc:	Critical Volume

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