L-Norleucine, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi: InChI=1S/C14H27NO4/c1-6-8-9-12(15-14(17)18-7-2)13(16)19-11(5)10(3)4/h10-12H,6-9H

InchiKey: UEAALMGOTGPLJC-JHJMLUEUSA-N

Formula: C14H27NO4

SMILES: CCCCC(NC(=O)OCC)C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 273.37

Physical Properties

Property code	Value	Unit	Source
gf	-318.77	kJ/mol	Joback Method
hf	-784.26	kJ/mol	Joback Method
hfus	32.12	kJ/mol	Joback Method
hvap	70.34	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.879		Crippen Method
mcvol	232.980	ml/mol	McGowan Method
pc	1689.34	kPa	Joback Method
rinpol	1704.70		NIST Webbook
rinpol	1704.70		NIST Webbook
tb	721.15	K	Joback Method
tc	907.25	K	Joback Method
tf	399.52	K	Joback Method
vc	0.884	m3/kmol	Joback Method

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

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=R502146&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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