D-Leucine, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi: InChI=1S/C14H27NO4/c1-7-18-14(17)15-12(8-9(2)3)13(16)19-11(6)10(4)5/h9-12H,7-8H2

InchiKey: UJEQPEHLZYHWJT-JHJMLUEUSA-N

Formula: C14H27NO4

SMILES: CCOC(=O)NC(CC(C)C)C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 273.37

Physical Properties

Property code	Value	Unit	Source
gf	-321.21	kJ/mol	Joback Method
hf	-789.54	kJ/mol	Joback Method
hfus	28.60	kJ/mol	Joback Method
hvap	69.95	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.735		Crippen Method
mcvol	232.980	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
rinpol	1638.10		NIST Webbook
rinpol	1638.10		NIST Webbook
tb	720.71	K	Joback Method
tc	909.23	K	Joback Method
tf	384.52	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.96	J/mol×K	720.71	Joback Method
cpg	699.14	J/mol×K	752.13	Joback Method
cpg	714.43	J/mol×K	783.55	Joback Method
cpg	728.81	J/mol×K	814.97	Joback Method
cpg	742.31	J/mol×K	846.39	Joback Method
cpg	754.92	J/mol×K	877.81	Joback Method
cpg	766.65	J/mol×K	909.23	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=R501861&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume