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

Inchi: InChI=1S/C13H25NO4/c1-7-17-13(16)14-11(9(4)5)12(15)18-10(6)8(2)3/h8-11H,7H2,1-6H

InchiKey: ZYEHEHZLKTWBIM-VUWPPUDQSA-N

Formula: C13H25NO4

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

Mol. weight [g/mol]: 259.34

Physical Properties

Property code	Value	Unit	Source
gf	-329.63	kJ/mol	Joback Method
hf	-768.90	kJ/mol	Joback Method
hfus	26.01	kJ/mol	Joback Method
hvap	67.73	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.345		Crippen Method
mcvol	218.890	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	1584.80		NIST Webbook
rinpol	1584.80		NIST Webbook
tb	697.83	K	Joback Method
tc	887.34	K	Joback Method
tf	373.25	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.66	J/mol×K	697.83	Joback Method
cpg	643.47	J/mol×K	729.42	Joback Method
cpg	658.42	J/mol×K	761.00	Joback Method
cpg	672.52	J/mol×K	792.59	Joback Method
cpg	685.76	J/mol×K	824.17	Joback Method
cpg	698.15	J/mol×K	855.76	Joback Method
cpg	709.70	J/mol×K	887.34	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=R502235&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