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

Inchi: InChI=1S/C13H25NO4/c1-6-8-11(14-13(16)17-7-2)12(15)18-10(5)9(3)4/h9-11H,6-8H2,1-

InchiKey: SDTGTNCCGSTRES-NFJWQWPMSA-N

Formula: C13H25NO4

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

Mol. weight [g/mol]: 259.34

Physical Properties

Property code	Value	Unit	Source
gf	-327.19	kJ/mol	Joback Method
hf	-763.62	kJ/mol	Joback Method
hfus	29.53	kJ/mol	Joback Method
hvap	68.12	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.489		Crippen Method
mcvol	218.890	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	1605.50		NIST Webbook
rinpol	1617.40		NIST Webbook
rinpol	1605.50		NIST Webbook
tb	698.27	K	Joback Method
tc	885.10	K	Joback Method
tf	388.25	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.16	J/mol×K	698.27	Joback Method
cpg	642.73	J/mol×K	729.41	Joback Method
cpg	657.47	J/mol×K	760.55	Joback Method
cpg	671.38	J/mol×K	791.68	Joback Method
cpg	684.47	J/mol×K	822.82	Joback Method
cpg	696.74	J/mol×K	853.96	Joback Method
cpg	708.21	J/mol×K	885.10	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=R501905&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