

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

Inchi:	InChI=1S/C11H21NO4/c1-6-15-11(14)12-8(4)10(13)16-9(5)7(2)3/h7-9H,6H2,1-5H3,(H,12)
InchiKey:	SURZINZIGAZKED-GKAPJAKFSA-N
Formula:	C11H21NO4
SMILES:	CCOC(=O)NC(C)C(=O)OC(C)C(C)C
Mol. weight [g/mol]:	231.29

Physical Properties

Property code	Value	Unit	Source
gf	-344.03	kJ/mol	Joback Method
hf	-722.34	kJ/mol	Joback Method
hfus	24.35	kJ/mol	Joback Method
hvap	63.66	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.709		Crippen Method
mcvol	190.710	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	1473.30		NIST Webbook
rinpol	1473.30		NIST Webbook
tb	652.51	K	Joback Method
tc	842.10	K	Joback Method
tf	365.71	K	Joback Method
vc	0.717	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.32	J/molxK	652.51	Joback Method
cpg	534.94	J/molxK	684.11	Joback Method
cpg	548.82	J/molxK	715.71	Joback Method
cpg	561.96	J/molxK	747.30	Joback Method
cpg	574.35	J/molxK	778.90	Joback Method
cpg	586.01	J/molxK	810.50	Joback Method
cpg	596.92	J/molxK	842.10	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=R502037&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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

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