

# D-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	1458.30		NIST Webbook
rinpol	1458.30		NIST Webbook
tb	652.51	K	Joback Method
tc	842.10	K	Joback Method
tf	365.71	K	Joback Method
vc	0.717	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.32	J/mol×K	652.51	Joback Method
cpg	534.94	J/mol×K	684.11	Joback Method
cpg	548.82	J/mol×K	715.71	Joback Method
cpg	561.96	J/mol×K	747.30	Joback Method
cpg	574.35	J/mol×K	778.90	Joback Method
cpg	586.01	J/mol×K	810.50	Joback Method
cpg	596.92	J/mol×K	842.10	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R501787&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R501787&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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