

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

<b>Inchi:</b>	InChI=1S/C13H25NO4S/c1-6-17-13(16)14-11(7-8-19-5)12(15)18-10(4)9(2)3/h9-11H,6-8H
<b>InchiKey:</b>	MICKYEAKDKWODH-NFJWQWPMISA-N
<b>Formula:</b>	C13H25NO4S
<b>SMILES:</b>	CCOC(=O)NC(CCSC)C(=O)OC(C)C(C)C
<b>Mol. weight [g/mol]:</b>	291.41

## Physical Properties

Property code	Value	Unit	Source
gf	-294.07	kJ/mol	Joback Method
hf	-721.75	kJ/mol	Joback Method
hfus	33.66	kJ/mol	Joback Method
hvap	74.93	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.442		Crippen Method
mvol	235.240	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	1914.20		NIST Webbook
rinpol	1914.20		NIST Webbook
tb	767.05	K	Joback Method
tc	967.58	K	Joback Method
tf	422.65	K	Joback Method
vc	0.882	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.93	J/molxK	767.05	Joback Method
cpg	701.87	J/molxK	800.47	Joback Method
cpg	715.80	J/molxK	833.89	Joback Method
cpg	728.72	J/molxK	867.32	Joback Method
cpg	740.65	J/molxK	900.74	Joback Method
cpg	751.57	J/molxK	934.16	Joback Method
cpg	761.49	J/molxK	967.58	Joback Method

# Sources

<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=R502131&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R502131&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>hvp:</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>rinp:</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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