

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

Inchi:	InChI=1S/C16H30N2O6/c1-6-22-15(20)17-10-8-9-13(18-16(21)23-7-2)14(19)24-12(5)11
InchiKey:	PKDJRCOUQAURDP-PZORYLMUSA-N
Formula:	C16H30N2O6
SMILES:	CCOC(=O)NCCCC(NC(=O)OCC)C(=O)OC(C)C(C)C
Mol. weight [g/mol]:	346.42

## Physical Properties

Property code	Value	Unit	Source
gf	-446.46	kJ/mol	Joback Method
hf	-1016.87	kJ/mol	Joback Method
hfus	45.19	kJ/mol	Joback Method
hvap	90.39	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.215		Crippen Method
mcvol	278.580	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
rinpol	2281.70		NIST Webbook
rinpol	2281.70		NIST Webbook
tb	893.37	K	Joback Method
tc	1096.44	K	Joback Method
tf	546.88	K	Joback Method
vc	1.056	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.14	J/molxK	893.37	Joback Method
cpg	917.05	J/molxK	927.22	Joback Method
cpg	929.71	J/molxK	961.06	Joback Method
cpg	941.12	J/molxK	994.91	Joback Method
cpg	951.30	J/molxK	1028.75	Joback Method
cpg	960.22	J/molxK	1062.60	Joback Method
cpg	967.91	J/molxK	1096.44	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.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>
<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=R502166&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R502166&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>hvpap:</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>rinppl:</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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