

# «beta»-Alanine, N-isobutyryl-, octyl ester

<b>Inchi:</b>	InChI=1S/C15H29NO3/c1-4-5-6-7-8-9-12-19-14(17)10-11-16-15(18)13(2)3/h13H,4-12H2
<b>InchiKey:</b>	FUOMJHAVSXSXSVHV-UHFFFAOYSA-N
<b>Formula:</b>	C15H29NO3
<b>SMILES:</b>	CCCCCCCCOC(=O)CCNC(=O)C(C)C
<b>Mol. weight [g/mol]:</b>	271.40

## Physical Properties

Property code	Value	Unit	Source
gf	-200.47	kJ/mol	Joback Method
hf	-662.12	kJ/mol	Joback Method
hfus	40.57	kJ/mol	Joback Method
hvap	70.93	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.052		Crippen Method
mvol	241.200	ml/mol	McGowan Method
pc	1564.75	kPa	Joback Method
rinpol	2015.00		NIST Webbook
rinpol	2015.00		NIST Webbook
tb	722.49	K	Joback Method
tc	903.63	K	Joback Method
tf	418.56	K	Joback Method
vc	0.934	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.39	J/mol×K	722.49	Joback Method
cpg	724.58	J/mol×K	752.68	Joback Method
cpg	739.93	J/mol×K	782.87	Joback Method
cpg	754.45	J/mol×K	813.06	Joback Method
cpg	768.17	J/mol×K	843.25	Joback Method
cpg	781.11	J/mol×K	873.44	Joback Method
cpg	793.27	J/mol×K	903.63	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=U321666&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321666&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>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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