

# «beta»-Alanine, N-caproyl-, butyl ester

<b>Inchi:</b>	InChI=1S/C13H25NO3/c1-3-5-7-8-12(15)14-10-9-13(16)17-11-6-4-2/h3-11H2,1-2H3,(H,1
<b>InchiKey:</b>	JFBCRSPRCVDTTI-UHFFFAOYSA-N
<b>Formula:</b>	C13H25NO3
<b>SMILES:</b>	CCCCC(=O)NCCC(=O)OCCCC
<b>Mol. weight [g/mol]:</b>	243.34

## Physical Properties

Property code	Value	Unit	Source
gf	-214.87	kJ/mol	Joback Method
hf	-615.56	kJ/mol	Joback Method
hfus	38.91	kJ/mol	Joback Method
hvap	66.87	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.416		Crippen Method
mvol	213.020	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	1872.00		NIST Webbook
rinpol	1872.00		NIST Webbook
tb	677.17	K	Joback Method
tc	856.53	K	Joback Method
tf	411.02	K	Joback Method
vc	0.829	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.44	J/mol×K	677.17	Joback Method
cpg	612.52	J/mol×K	707.06	Joback Method
cpg	626.87	J/mol×K	736.96	Joback Method
cpg	640.50	J/mol×K	766.85	Joback Method
cpg	653.42	J/mol×K	796.74	Joback Method
cpg	665.64	J/mol×K	826.64	Joback Method
cpg	677.17	J/mol×K	856.53	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=U321781&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321781&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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