

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

Inchi:	InChI=1S/C17H33NO3/c1-3-5-7-8-9-11-15-21-17(20)13-14-18-16(19)12-10-6-4-2/h3-15H
InchiKey:	MMBXCVDQCDHCKA-UHFFFAOYSA-N
Formula:	C17H33NO3
SMILES:	CCCCCCCCOC(=O)CCNC(=O)CCCCC
Mol. weight [g/mol]:	299.45

## Physical Properties

Property code	Value	Unit	Source
gf	-181.19	kJ/mol	Joback Method
hf	-698.12	kJ/mol	Joback Method
hfus	49.27	kJ/mol	Joback Method
hvap	75.77	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.977		Crippen Method
mcvol	269.380	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
rinpol	2273.00		NIST Webbook
rinpol	2273.00		NIST Webbook
tb	768.69	K	Joback Method
tc	949.75	K	Joback Method
tf	456.10	K	Joback Method
vc	1.052	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.82	J/molxK	768.69	Joback Method
cpg	839.64	J/molxK	798.87	Joback Method
cpg	855.55	J/molxK	829.04	Joback Method
cpg	870.59	J/molxK	859.22	Joback Method
cpg	884.78	J/molxK	889.40	Joback Method
cpg	898.13	J/molxK	919.58	Joback Method
cpg	910.67	J/molxK	949.75	Joback Method

# Sources

<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.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=U321785&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321785&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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