

# «beta»-Alanine, N-hexyloxycarbonyl-, hexyl ester

Inchi:	InChI=1S/C16H31NO4/c1-3-5-7-9-13-20-15(18)11-12-17-16(19)21-14-10-8-6-4-2/h3-14H
InchiKey:	AKHWUAIORNGQKP-UHFFFAOYSA-N
Formula:	C16H31NO4
SMILES:	CCCCCOC(=O)CCNC(=O)OCCCCC
Mol. weight [g/mol]:	301.42

## Physical Properties

Property code	Value	Unit	Source
gf	-294.61	kJ/mol	Joback Method
hf	-809.70	kJ/mol	Joback Method
hfus	47.87	kJ/mol	Joback Method
hvap	75.96	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.807		Crippen Method
mcvol	261.160	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook
tb	768.23	K	Joback Method
tc	949.61	K	Joback Method
tf	467.06	K	Joback Method
vc	1.014	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.81	J/mol×K	768.23	Joback Method
cpg	811.01	J/mol×K	798.46	Joback Method
cpg	826.31	J/mol×K	828.69	Joback Method
cpg	840.73	J/mol×K	858.92	Joback Method
cpg	854.29	J/mol×K	889.15	Joback Method
cpg	866.98	J/mol×K	919.38	Joback Method
cpg	878.83	J/mol×K	949.61	Joback Method

# Sources

<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=U393138&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393138&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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