

# «beta»-Alanine, N-(2-methylbenzoyl)-, isohexyl ester

<b>Inchi:</b>	InChI=1S/C17H25NO3/c1-13(2)7-6-12-21-16(19)10-11-18-17(20)15-9-5-4-8-14(15)3/h4-13
<b>InchiKey:</b>	SFVYAXVKCRHXKT-UHFFFAOYSA-N
<b>Formula:</b>	C17H25NO3
<b>SMILES:</b>	<chem>Cc1ccccc1C(=O)NCCCC(=O)OCCCC(C)C</chem>
<b>Mol. weight [g/mol]:</b>	291.39

## Physical Properties

Property code	Value	Unit	Source
gf	-80.85	kJ/mol	Joback Method
hf	-478.34	kJ/mol	Joback Method
hfus	39.40	kJ/mol	Joback Method
hvap	78.32	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.094		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinsol	2301.00		NIST Webbook
tb	799.91	K	Joback Method
tc	1005.41	K	Joback Method
tf	480.04	K	Joback Method
vc	0.939	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.88	J/mol×K	799.91	Joback Method
cpg	749.14	J/mol×K	834.16	Joback Method
cpg	763.35	J/mol×K	868.41	Joback Method
cpg	776.54	J/mol×K	902.66	Joback Method
cpg	788.75	J/mol×K	936.91	Joback Method
cpg	800.01	J/mol×K	971.16	Joback Method
cpg	810.35	J/mol×K	1005.41	Joback Method

# Sources

<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=U321616&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321616&amp;Units=SI</a>
<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>

# 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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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