

# «beta»-Alanine, N-(4-butylbenzoyl)-, isohexyl ester

Inchi:	InChI=1S/C20H31NO3/c1-4-5-8-17-9-11-18(12-10-17)20(23)21-14-13-19(22)24-15-6-7-1
InchiKey:	REGBGZOAQLTASJ-UHFFFAOYSA-N
Formula:	C20H31NO3
SMILES:	CCCCc1ccc(C(=O)NCCCC(=O)OCCCC(C)C)cc1
Mol. weight [g/mol]:	333.46

## Physical Properties

Property code	Value	Unit	Source
gf	-55.59	kJ/mol	Joback Method
hf	-540.26	kJ/mol	Joback Method
hfus	47.17	kJ/mol	Joback Method
hvap	85.00	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.128		Crippen Method
mvol	287.890	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
rinpol	2683.00		NIST Webbook
rinpol	2683.00		NIST Webbook
tb	868.55	K	Joback Method
tc	1073.74	K	Joback Method
tf	513.85	K	Joback Method
vc	1.107	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.49	J/mol×K	868.55	Joback Method
cpg	924.40	J/mol×K	902.75	Joback Method
cpg	939.17	J/mol×K	936.95	Joback Method
cpg	952.84	J/mol×K	971.14	Joback Method
cpg	965.45	J/mol×K	1005.34	Joback Method
cpg	977.04	J/mol×K	1039.54	Joback Method
cpg	987.66	J/mol×K	1073.74	Joback Method

# Sources

<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=U321772&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321772&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>h vap:</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>r in pol:</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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