

# «beta»-Alanine, N-(2-bromobenzoyl)-, butyl ester

Inchi:	InChI=1S/C14H18BrNO3/c1-2-3-10-19-13(17)8-9-16-14(18)11-6-4-5-7-12(11)15/h4-7H,2
InchiKey:	YCNWIVIRWNVMSN-UHFFFAOYSA-N
Formula:	C14H18BrNO3
SMILES:	CCCCOC(=O)CCNC(=O)c1ccccc1Br
Mol. weight [g/mol]:	328.20

## Physical Properties

Property code	Value	Unit	Source
gf	-89.35	kJ/mol	Joback Method
hf	-384.81	kJ/mol	Joback Method
hfus	40.44	kJ/mol	Joback Method
hvap	78.47	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	2.912		Crippen Method
mcvol	220.850	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpola	2340.00		NIST Webbook
rinpola	2340.00		NIST Webbook
tb	797.87	K	Joback Method
tc	1015.73	K	Joback Method
tf	521.03	K	Joback Method
vc	0.839	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.80	J/mol×K	797.87	Joback Method
cpg	616.38	J/mol×K	834.18	Joback Method
cpg	628.03	J/mol×K	870.49	Joback Method
cpg	638.78	J/mol×K	906.80	Joback Method
cpg	648.68	J/mol×K	943.11	Joback Method
cpg	657.75	J/mol×K	979.42	Joback Method
cpg	666.03	J/mol×K	1015.73	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321728&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321728&amp;Units=SI</a>
<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>

# 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>hvpap:</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>rinppl:</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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