

# «beta»-Alanine, N-(3-bromobenzoyl)-, ethyl ester

Inchi:	InChI=1S/C12H14BrNO3/c1-2-17-11(15)6-7-14-12(16)9-4-3-5-10(13)8-9/h3-5,8H,2,6-7H
InchiKey:	NMGLDLCSHSHWHY-UHFFFAOYSA-N
Formula:	C12H14BrNO3
SMILES:	CCOC(=O)CCNC(=O)c1cccc(Br)c1
Mol. weight [g/mol]:	300.15

## Physical Properties

Property code	Value	Unit	Source
gf	-106.19	kJ/mol	Joback Method
hf	-343.53	kJ/mol	Joback Method
hfus	35.26	kJ/mol	Joback Method
hvap	74.02	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.132		Crippen Method
mcvol	192.670	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
rinpola	2171.00		NIST Webbook
rinpola	2171.00		NIST Webbook
tb	752.11	K	Joback Method
tc	975.87	K	Joback Method
tf	498.49	K	Joback Method
vc	0.727	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.89	J/mol×K	752.11	Joback Method
cpg	508.65	J/mol×K	789.40	Joback Method
cpg	519.52	J/mol×K	826.70	Joback Method
cpg	529.54	J/mol×K	863.99	Joback Method
cpg	538.74	J/mol×K	901.28	Joback Method
cpg	547.14	J/mol×K	938.57	Joback Method
cpg	554.79	J/mol×K	975.87	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=U321637&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321637&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>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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