

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

Inchi:	InChI=1S/C19H28BrNO3/c1-2-3-4-5-6-7-10-15-24-18(22)13-14-21-19(23)16-11-8-9-12-1
InchiKey:	WRGDPYMABLDIMC-UHFFFAOYSA-N
Formula:	C19H28BrNO3
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)c1ccccc1Br
Mol. weight [g/mol]:	398.33

## Physical Properties

Property code	Value	Unit	Source
gf	-47.25	kJ/mol	Joback Method
hf	-488.01	kJ/mol	Joback Method
hfus	53.39	kJ/mol	Joback Method
hvap	89.60	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	4.863		Crippen Method
mcvol	291.300	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
rinsol	2897.00		NIST Webbook
tb	912.27	K	Joback Method
tc	1126.24	K	Joback Method
tf	577.38	K	Joback Method
vc	1.119	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.92	J/mol×K	912.27	Joback Method
cpg	901.92	J/mol×K	947.93	Joback Method
cpg	914.87	J/mol×K	983.59	Joback Method
cpg	926.82	J/mol×K	1019.25	Joback Method
cpg	937.82	J/mol×K	1054.91	Joback Method
cpg	947.93	J/mol×K	1090.58	Joback Method
cpg	957.18	J/mol×K	1126.24	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=U321733&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321733&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>
<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>

# 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>mccvol:</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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