

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

Inchi:	InChI=1S/C21H32BrNO3/c1-2-3-4-5-6-7-8-9-12-17-26-20(24)15-16-23-21(25)18-13-10-1
InchiKey:	WQDHVPAEIOKYRO-UHFFFAOYSA-N
Formula:	C21H32BrNO3
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)c1ccccc1Br
Mol. weight [g/mol]:	426.39

## Physical Properties

Property code	Value	Unit	Source
gf	-30.41	kJ/mol	Joback Method
hf	-529.29	kJ/mol	Joback Method
hfus	58.57	kJ/mol	Joback Method
hvap	94.05	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	5.643		Crippen Method
mcvol	319.480	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
rinpol	3250.00		NIST Webbook
rinpol	3250.00		NIST Webbook
tb	958.03	K	Joback Method
tc	1175.76	K	Joback Method
tf	599.92	K	Joback Method
vc	1.230	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.97	J/molxK	958.03	Joback Method
cpg	1021.50	J/molxK	994.32	Joback Method
cpg	1034.91	J/molxK	1030.61	Joback Method
cpg	1047.27	J/molxK	1066.90	Joback Method
cpg	1058.62	J/molxK	1103.18	Joback Method
cpg	1069.04	J/molxK	1139.47	Joback Method
cpg	1078.59	J/molxK	1175.76	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=U321735&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321735&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>

# 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>hvp:</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>rinp:</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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