

# L-Valine, N-(3-bromobenzoyl)-, nonyl ester

<b>Inchi:</b>	InChI=1S/C21H32BrNO3/c1-4-5-6-7-8-9-10-14-26-21(25)19(16(2)3)23-20(24)17-12-11-1
<b>InchiKey:</b>	DHWILQRKPMRJJN-UHFFFAOYSA-N
<b>Formula:</b>	C21H32BrNO3
<b>SMILES:</b>	CCCCCCCCCOC(=O)C(NC(=O)c1cccc(Br)c1)C(C)C
<b>Mol. weight [g/mol]:</b>	426.39

## Physical Properties

Property code	Value	Unit	Source
gf	-35.29	kJ/mol	Joback Method
hf	-539.85	kJ/mol	Joback Method
hfus	51.52	kJ/mol	Joback Method
hvap	93.27	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	5.497		Crippen Method
mvol	319.480	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	2847.00		NIST Webbook
rinpol	2847.00		NIST Webbook
tb	957.15	K	Joback Method
tc	1176.87	K	Joback Method
tf	569.92	K	Joback Method
vc	1.218	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1007.83	J/molxK	957.15	Joback Method
cpg	1022.39	J/molxK	993.77	Joback Method
cpg	1035.78	J/molxK	1030.39	Joback Method
cpg	1048.07	J/molxK	1067.01	Joback Method
cpg	1059.32	J/molxK	1103.63	Joback Method
cpg	1069.59	J/molxK	1140.25	Joback Method
cpg	1078.94	J/molxK	1176.87	Joback Method

# Sources

<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.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>
<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=U346691&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346691&amp;Units=SI</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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