

# L-Valine, N-(3-trifluoromethylbenzoyl)-, butyl ester

<b>Inchi:</b>	InChI=1S/C17H22F3NO3/c1-4-5-9-24-16(23)14(11(2)3)21-15(22)12-7-6-8-13(10-12)17(1)
<b>InchiKey:</b>	UXDWHIXAPWDPCO-UHFFFAOYSA-N
<b>Formula:</b>	C17H22F3NO3
<b>SMILES:</b>	CCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1)C(C)C
<b>Mol. weight [g/mol]:</b>	345.36

## Physical Properties

Property code	Value	Unit	Source
gf	-664.88	kJ/mol	Joback Method
hf	-1080.70	kJ/mol	Joback Method
hfus	37.70	kJ/mol	Joback Method
hvap	74.19	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	3.803		Crippen Method
mvol	250.930	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	1992.00		NIST Webbook
rinpol	1992.00		NIST Webbook
tb	794.05	K	Joback Method
tc	991.72	K	Joback Method
tf	469.23	K	Joback Method
vc	0.976	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.76	J/molxK	794.05	Joback Method
cpg	772.89	J/molxK	827.00	Joback Method
cpg	786.04	J/molxK	859.94	Joback Method
cpg	798.24	J/molxK	892.89	Joback Method
cpg	809.55	J/molxK	925.83	Joback Method
cpg	820.02	J/molxK	958.78	Joback Method
cpg	829.68	J/molxK	991.72	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U346716&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346716&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>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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