

# L-Valine, N-pentafluorobenzoyl-, nonyl ester

**Inchi:** InChI=1S/C21H28F5NO3/c1-4-5-6-7-8-9-10-11-30-21(29)19(12(2)3)27-20(28)13-14(22)1  
**InchiKey:** RMXWJBJYVSEFRG-UHFFFAOYSA-N  
**Formula:** C21H28F5NO3  
**SMILES:** CCCCCCCCCOC(=O)C(NC(=O)c1c(F)c(F)c(F)c(F)c1F)C(C)C  
**Mol. weight [g/mol]:** 437.44

## Physical Properties

Property code	Value	Unit	Source
gf	-1062.18	kJ/mol	Joback Method
hf	-1592.61	kJ/mol	Joback Method
hfus	60.08	kJ/mol	Joback Method
hvap	85.40	kJ/mol	Joback Method
log10ws	-7.65		Crippen Method
logp	5.430		Crippen Method
mvol	310.830	ml/mol	McGowan Method
pc	1064.48	kPa	Joback Method
rinpol	2391.00		NIST Webbook
rinpol	2391.00		NIST Webbook
tb	907.26	K	Joback Method
tc	1110.82	K	Joback Method
tf	563.15	K	Joback Method
vc	1.246	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.48	J/molxK	907.26	Joback Method
cpg	1016.16	J/molxK	941.19	Joback Method
cpg	1029.68	J/molxK	975.11	Joback Method
cpg	1042.05	J/molxK	1009.04	Joback Method
cpg	1053.30	J/molxK	1042.96	Joback Method
cpg	1063.45	J/molxK	1076.89	Joback Method
cpg	1072.53	J/molxK	1110.82	Joback Method

# Sources

<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=U346610&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346610&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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