

# L-Valine, N-(3-fluoro-4-trifluoromethylbenzoyl)-, undecyl ester

InChI: InChI=1S/C24H35F4NO3/c1-4-5-6-7-8-9-10-11-12-15-32-23(31)21(17(2)3)29-22(30)18-1  
InChIKey: AXQLAVYIOPRZID-UHFFFAOYSA-N

Formula: C24H35F4NO3

SMILES: CCCCCCCCCCOC(=O)C(NC(=O)c1ccc(C(F)(F)F)c(F)c1)C(C)C

Mol. weight [g/mol]: 461.53

## Physical Properties

Property code	Value	Unit	Source
gf	-810.38	kJ/mol	Joback Method
hf	-1432.76	kJ/mol	Joback Method
hfus	58.52	kJ/mol	Joback Method
hvap	89.62	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	6.673		Crippen Method
mcvol	351.330	ml/mol	McGowan Method
pc	950.25	kPa	Joback Method
rinpol	2562.00		NIST Webbook
rinpol	2562.00		NIST Webbook
tb	958.46	K	Joback Method
tc	1174.15	K	Joback Method
tf	561.23	K	Joback Method
vc	1.385	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1178.66	J/molxK	958.46	Joback Method
cpg	1194.77	J/molxK	994.41	Joback Method
cpg	1209.63	J/molxK	1030.36	Joback Method
cpg	1223.31	J/molxK	1066.31	Joback Method
cpg	1235.90	J/molxK	1102.25	Joback Method
cpg	1247.47	J/molxK	1138.20	Joback Method
cpg	1258.10	J/molxK	1174.15	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=U346560&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346560&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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