

# L-Valine, N-(2-trifluoromethylbenzoyl)-, pentadecyl ester

<b>Inchi:</b>	InChI=1S/C28H44F3NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-21-35-27(34)25(22(2)3)3
<b>InchiKey:</b>	GAFGJEFPXOEBJK-UHFFFAOYSA-N
<b>Formula:</b>	C28H44F3NO3
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1ccccc1C(F)(F)F)C(C)C
<b>Mol. weight [g/mol]:</b>	499.65

## Physical Properties

Property code	Value	Unit	Source
gf	-572.26	kJ/mol	Joback Method
hf	-1307.74	kJ/mol	Joback Method
hfus	66.19	kJ/mol	Joback Method
hvap	98.67	kJ/mol	Joback Method
log10ws	-9.61		Crippen Method
logp	8.094		Crippen Method
mcvol	405.920	ml/mol	McGowan Method
pc	785.51	kPa	Joback Method
rinpol	3139.00		NIST Webbook
rinpol	3139.00		NIST Webbook
tb	1045.73	K	Joback Method
tc	1290.61	K	Joback Method
tf	593.20	K	Joback Method
vc	1.591	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1422.02	J/molxK	1045.73	Joback Method
cpg	1440.35	J/molxK	1086.54	Joback Method
cpg	1457.16	J/molxK	1127.36	Joback Method
cpg	1472.59	J/molxK	1168.17	Joback Method
cpg	1486.79	J/molxK	1208.98	Joback Method
cpg	1499.88	J/molxK	1249.80	Joback Method
cpg	1512.02	J/molxK	1290.61	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U346714&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346714&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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