

# L-Valine, N-(2-fluoro-3-trifluoromethylbenzoyl)-, tetradecyl ester

InChI: CCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1F)C(C)C  
InChIKey: KDXUKKURNXLCEJ-UHFFFAOYSA-N

Formula: C<sub>27</sub>H<sub>41</sub>F<sub>4</sub>NO<sub>3</sub>

SMILES: CCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1F)C(C)C

Mol. weight [g/mol]: 503.61

## Physical Properties

Property code	Value	Unit	Source
gf	-785.12	kJ/mol	Joback Method
hf	-1494.68	kJ/mol	Joback Method
hfus	66.29	kJ/mol	Joback Method
hvap	96.29	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	7.843		Crippen Method
mvol	393.600	ml/mol	McGowan Method
pc	801.60	kPa	Joback Method
rinpol	2940.00		NIST Webbook
rinpol	2940.00		NIST Webbook
tb	1027.10	K	Joback Method
tc	1267.19	K	Joback Method
tf	595.04	K	Joback Method
vc	1.554	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1364.84	J/mol×K	1027.10	Joback Method
cpg	1382.55	J/mol×K	1067.11	Joback Method
cpg	1398.74	J/mol×K	1107.13	Joback Method
cpg	1413.54	J/mol×K	1147.14	Joback Method
cpg	1427.07	J/mol×K	1187.16	Joback Method
cpg	1439.46	J/mol×K	1227.17	Joback Method
cpg	1450.82	J/mol×K	1267.19	Joback Method

# Sources

<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=U346474&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346474&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>h vap:</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>r in pol:</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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