

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

InChI: InChI=1S/C30H47F4NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-38-29(37)27(28)19-20-21-26-25-24-23  
InChIKey: XUTXJSFAUWAQAZ-UHFFFAOYSA-N

Formula: C30H47F4NO3

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

Mol. weight [g/mol]: 545.69

## Physical Properties

Property code	Value	Unit	Source
gf	-759.86	kJ/mol	Joback Method
hf	-1556.60	kJ/mol	Joback Method
hfus	74.06	kJ/mol	Joback Method
hvap	102.97	kJ/mol	Joback Method
log10ws	-10.77		Crippen Method
logp	9.014		Crippen Method
mvol	435.870	ml/mol	McGowan Method
pc	685.29	kPa	Joback Method
rinpol	3258.00		NIST Webbook
rinpol	3258.00		NIST Webbook
tb	1095.74	K	Joback Method
tc	1372.53	K	Joback Method
tf	628.85	K	Joback Method
vc	1.722	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1554.86	J/molxK	1095.74	Joback Method
cpg	1574.73	J/molxK	1141.87	Joback Method
cpg	1592.72	J/molxK	1188.00	Joback Method
cpg	1609.04	J/molxK	1234.13	Joback Method
cpg	1623.89	J/molxK	1280.26	Joback Method
cpg	1637.49	J/molxK	1326.40	Joback Method
cpg	1650.03	J/molxK	1372.53	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U346477&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346477&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>hvpap:</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>rinppl:</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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