

# L-Valine, N-(2-fluoro-6-trifluoromethylbenzoyl)-, hexadecyl ester

InChI: InChI=1S/C29H45F4NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-37-28(36)26(22(23)24)25  
InChIKey: RXJBXHYUBPUVIW-UHFFFAOYSA-N

Formula: C29H45F4NO3

SMILES: CCCCCCCCCCCCCCOC(=O)C(NC(=O)c1c(F)ccc1C(F)(F)F)C(C)C

Mol. weight [g/mol]: 531.67

## Physical Properties

Property code	Value	Unit	Source
gf	-768.28	kJ/mol	Joback Method
hf	-1535.96	kJ/mol	Joback Method
hfus	71.47	kJ/mol	Joback Method
hvap	100.75	kJ/mol	Joback Method
log10ws	-10.36		Crippen Method
logp	8.623		Crippen Method
mcvol	421.780	ml/mol	McGowan Method
pc	721.08	kPa	Joback Method
rinpol	3243.00		NIST Webbook
rinpol	3243.00		NIST Webbook
tb	1072.86	K	Joback Method
tc	1335.87	K	Joback Method
tf	617.58	K	Joback Method
vc	1.665	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1491.15	J/molxK	1072.86	Joback Method
cpg	1510.22	J/molxK	1116.69	Joback Method
cpg	1527.55	J/molxK	1160.53	Joback Method
cpg	1543.30	J/molxK	1204.36	Joback Method
cpg	1557.66	J/molxK	1248.20	Joback Method
cpg	1570.78	J/molxK	1292.03	Joback Method
cpg	1582.85	J/molxK	1335.87	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U346497&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346497&amp;Units=SI</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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