

# L-Valine, N-(5-fluoro-2-trifluoromethyl)-, octadecyl ester

Inchi:	InChI=1S/C31H49F4NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-39-30(38)2
InchiKey:	XKZWYJAYBYIJNH-UHFFFAOYSA-N
Formula:	C31H49F4NO3
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cc(F)ccc1C(F)(F)F)C(C)C
Mol. weight [g/mol]:	559.72

## Physical Properties

Property code	Value	Unit	Source
gf	-751.44	kJ/mol	Joback Method
hf	-1577.24	kJ/mol	Joback Method
hfus	76.65	kJ/mol	Joback Method
hvap	105.20	kJ/mol	Joback Method
log10ws	-11.19		Crippen Method
logp	9.404		Crippen Method
mcvol	449.960	ml/mol	McGowan Method
pc	652.10	kPa	Joback Method
rinpol	3355.00		NIST Webbook
rinpol	3355.00		NIST Webbook
tb	1118.62	K	Joback Method
tc	1410.90	K	Joback Method
tf	640.12	K	Joback Method
vc	1.778	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1618.91	J/molxK	1118.62	Joback Method
cpg	1639.67	J/molxK	1167.33	Joback Method
cpg	1658.40	J/molxK	1216.05	Joback Method
cpg	1675.35	J/molxK	1264.76	Joback Method
cpg	1690.78	J/molxK	1313.47	Joback Method
cpg	1704.93	J/molxK	1362.18	Joback Method
cpg	1718.07	J/molxK	1410.90	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.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>
<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=U346431&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346431&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>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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