

# L-Valine, N-(3-fluorobenzoyl)-, octadecyl ester

<b>Inchi:</b>	InChI=1S/C30H50FNO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-35-30(34)28
<b>InchiKey:</b>	CXRQMNYNRBIPFB-UHFFFAOYSA-N
<b>Formula:</b>	C30H50FNO3
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(F)c1)C(C)C
<b>Mol. weight [g/mol]:</b>	491.72

## Physical Properties

Property code	Value	Unit	Source
gf	-168.64	kJ/mol	Joback Method
hf	-948.05	kJ/mol	Joback Method
hfus	72.63	kJ/mol	Joback Method
hvap	106.06	kJ/mol	Joback Method
log10ws	-10.09		Crippen Method
logp	8.385		Crippen Method
mcvol	430.560	ml/mol	McGowan Method
pc	734.82	kPa	Joback Method
rinpol	3456.00		NIST Webbook
rinpol	3456.00		NIST Webbook
tb	1096.18	K	Joback Method
tc	1361.73	K	Joback Method
tf	612.14	K	Joback Method
vc	1.679	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1536.44	J/molxK	1096.18	Joback Method
cpg	1555.67	J/molxK	1140.44	Joback Method
cpg	1572.91	J/molxK	1184.70	Joback Method
cpg	1588.31	J/molxK	1228.96	Joback Method
cpg	1602.02	J/molxK	1273.21	Joback Method
cpg	1614.20	J/molxK	1317.47	Joback Method
cpg	1624.98	J/molxK	1361.73	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=U346684&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346684&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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