

# L-Valine, N-(3-methoxy-2,4,5-trifluorobenzoyl)-, octadecyl ester

Inchi: InChI=1S/C31H50F3NO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-39-31(37)  
InchiKey: FTUQLVUDOYBCDI-UHFFFAOYSA-N

Formula: C31H50F3NO4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cc(F)c(F)c(OC)c1F)C(C)C

Mol. weight [g/mol]: 557.73

## Physical Properties

Property code	Value	Unit	Source
gf	-683.73	kJ/mol	Joback Method
hf	-1527.54	kJ/mol	Joback Method
hfus	81.40	kJ/mol	Joback Method
hvap	111.05	kJ/mol	Joback Method
log10ws	-10.87		Crippen Method
logp	8.672		Crippen Method
mvol	454.060	ml/mol	McGowan Method
pc	645.16	kPa	Joback Method
rinpol	3597.00		NIST Webbook
rinpol	3597.00		NIST Webbook
tb	1154.96	K	Joback Method
tc	1472.47	K	Joback Method
tf	684.38	K	Joback Method
vc	1.788	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1635.16	J/molxK	1154.96	Joback Method
cpg	1652.85	J/molxK	1207.88	Joback Method
cpg	1667.12	J/molxK	1260.80	Joback Method
cpg	1678.14	J/molxK	1313.71	Joback Method
cpg	1686.06	J/molxK	1366.63	Joback Method
cpg	1691.05	J/molxK	1419.55	Joback Method
cpg	1693.27	J/molxK	1472.47	Joback Method

# Sources

<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=U346442&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346442&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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