

# L-Valine, N-(3,4-difluorobenzoyl)-, octadecyl ester

Inchi:	InChI=1S/C30H49F2NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-36-30(35)2
InchiKey:	NBOCEXRNQMJSJJI-UHFFFAOYSA-N
Formula:	C30H49F2NO3
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1ccc(F)c(F)c1)C(C)C
Mol. weight [g/mol]:	509.71

## Physical Properties

Property code	Value	Unit	Source
gf	-373.08	kJ/mol	Joback Method
hf	-1155.63	kJ/mol	Joback Method
hfus	75.32	kJ/mol	Joback Method
hvap	105.90	kJ/mol	Joback Method
log10ws	-10.42		Crippen Method
logp	8.524		Crippen Method
mvol	432.330	ml/mol	McGowan Method
pc	711.49	kPa	Joback Method
rinpol	3444.00		NIST Webbook
rinpol	3444.00		NIST Webbook
tb	1100.43	K	Joback Method
tc	1373.90	K	Joback Method
tf	625.25	K	Joback Method
vc	1.696	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1541.88	J/molxK	1100.43	Joback Method
cpg	1561.13	J/molxK	1146.01	Joback Method
cpg	1578.22	J/molxK	1191.59	Joback Method
cpg	1593.32	J/molxK	1237.16	Joback Method
cpg	1606.56	J/molxK	1282.74	Joback Method
cpg	1618.11	J/molxK	1328.32	Joback Method
cpg	1628.11	J/molxK	1373.90	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=U346514&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346514&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.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>

# 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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