

# L-Valine, N-(2,4-difluorobenzoyl)-, dodecyl ester

Inchi:	InChI=1S/C24H37F2NO3/c1-4-5-6-7-8-9-10-11-12-13-16-30-24(29)22(18(2)3)27-23(28)2
InchiKey:	LXEUVTIFSZDHGG-UHFFFAOYSA-N
Formula:	C24H37F2NO3
SMILES:	CCCCCCCCCCCCOC(=O)C(NC(=O)c1ccc(F)cc1F)C(C)C
Mol. weight [g/mol]:	425.55

## Physical Properties

Property code	Value	Unit	Source
gf	-423.60	kJ/mol	Joback Method
hf	-1031.79	kJ/mol	Joback Method
hfus	59.78	kJ/mol	Joback Method
hvap	92.55	kJ/mol	Joback Method
log10ws	-7.91		Crippen Method
logp	6.183		Crippen Method
mcvol	347.790	ml/mol	McGowan Method
pc	993.25	kPa	Joback Method
rinpol	2767.00		NIST Webbook
rinpol	2767.00		NIST Webbook
tb	963.15	K	Joback Method
tc	1179.39	K	Joback Method
tf	557.63	K	Joback Method
vc	1.361	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1164.78	J/molxK	963.15	Joback Method
cpg	1181.20	J/molxK	999.19	Joback Method
cpg	1196.25	J/molxK	1035.23	Joback Method
cpg	1210.00	J/molxK	1071.27	Joback Method
cpg	1222.49	J/molxK	1107.31	Joback Method
cpg	1233.78	J/molxK	1143.35	Joback Method
cpg	1243.93	J/molxK	1179.39	Joback Method

# Sources

<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=U346444&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346444&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>

# 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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