

# L-Valine, N-(2,5-difluorobenzoyl)-, isohexyl ester

<b>Inchi:</b>	InChI=1S/C18H25F2NO3/c1-11(2)6-5-9-24-18(23)16(12(3)4)21-17(22)14-10-13(19)7-8-1
<b>InchiKey:</b>	DIAVCUFXUMIAHQ-UHFFFAOYSA-N
<b>Formula:</b>	C18H25F2NO3
<b>SMILES:</b>	CC(C)CCCOC(=O)C(NC(=O)c1cc(F)ccc1F)C(C)C
<b>Mol. weight [g/mol]:</b>	341.39

## Physical Properties

Property code	Value	Unit	Source
gf	-476.56	kJ/mol	Joback Method
hf	-913.23	kJ/mol	Joback Method
hfus	40.71	kJ/mol	Joback Method
hvap	78.80	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	3.699		Crippen Method
mvol	263.250	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	2138.00		NIST Webbook
rinpol	2138.00		NIST Webbook
tb	825.43	K	Joback Method
tc	1025.25	K	Joback Method
tf	475.01	K	Joback Method
vc	1.018	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	806.43	J/mol×K	825.43	Joback Method
cpg	821.19	J/mol×K	858.73	Joback Method
cpg	834.91	J/mol×K	892.04	Joback Method
cpg	847.61	J/mol×K	925.34	Joback Method
cpg	859.33	J/mol×K	958.65	Joback Method
cpg	870.08	J/mol×K	991.95	Joback Method
cpg	879.91	J/mol×K	1025.25	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=U346458&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346458&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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