

# DL-Valine, N-methyl-N-hexyloxycarbonyl-, nonyl ester

<b>Inchi:</b>	InChI=1S/C22H43NO4/c1-6-8-10-12-13-14-16-17-26-21(24)20(19(3)4)23(5)22(25)27-18
<b>InchiKey:</b>	IVTACBNDVRVDOX-UHFFFAOYSA-N
<b>Formula:</b>	C22H43NO4
<b>SMILES:</b>	CCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	385.58

## Physical Properties

Property code	Value	Unit	Source
gf	-227.58	kJ/mol	Joback Method
hf	-930.04	kJ/mol	Joback Method
hfus	54.28	kJ/mol	Joback Method
hvap	84.15	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.954		Crippen Method
mvol	345.700	ml/mol	McGowan Method
pc	962.08	kPa	Joback Method
rinpol	2434.00		NIST Webbook
rinpol	2434.00		NIST Webbook
tb	866.90	K	Joback Method
tc	1061.39	K	Joback Method
tf	484.49	K	Joback Method
vc	1.321	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.05	J/molxK	866.90	Joback Method
cpg	1156.38	J/molxK	899.32	Joback Method
cpg	1174.44	J/molxK	931.73	Joback Method
cpg	1191.26	J/molxK	964.15	Joback Method
cpg	1206.88	J/molxK	996.56	Joback Method
cpg	1221.34	J/molxK	1028.98	Joback Method
cpg	1234.66	J/molxK	1061.39	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=U392892&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392892&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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