

# I-Norvaline, N-isobutoxycarbonyl-, tetradecyl ester

Inchi:	InChI=1S/C24H47NO4/c1-5-7-8-9-10-11-12-13-14-15-16-17-19-28-23(26)22(18-6-2)25-2
InchiKey:	XUBKZBMNDFIXLE-UHFFFAOYSA-N
Formula:	C24H47NO4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(CCC)NC(=O)OCC(C)C
Mol. weight [g/mol]:	413.63

## Physical Properties

Property code	Value	Unit	Source
gf	-232.13	kJ/mol	Joback Method
hf	-985.38	kJ/mol	Joback Method
hfus	61.54	kJ/mol	Joback Method
hvap	92.99	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	6.782		Crippen Method
mcvol	373.880	ml/mol	McGowan Method
pc	864.54	kPa	Joback Method
rinpol	2445.00		NIST Webbook
tb	950.39	K	Joback Method
tc	1166.86	K	Joback Method
tf	527.22	K	Joback Method
vc	1.450	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1284.03	J/molxK	950.39	Joback Method
cpg	1303.59	J/molxK	986.47	Joback Method
cpg	1321.56	J/molxK	1022.55	Joback Method
cpg	1337.96	J/molxK	1058.63	Joback Method
cpg	1352.86	J/molxK	1094.71	Joback Method
cpg	1366.28	J/molxK	1130.78	Joback Method
cpg	1378.28	J/molxK	1166.86	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=U320722&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320722&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>
<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

Latest version available from:

<https://www.chemeo.com/cid/58-561-5/l-Norvaline-N-isobutoxycarbonyl-tetradecyl-ester.pdf>

Generated by Cheméo on 2024-04-24 19:29:59.085288485 +0000 UTC m=+16276248.005865798.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.