

L-Norvaline, N-isobutoxycarbonyl-, heptadecyl ester

Inchi:	InChI=1S/C27H53NO4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22-31-26(29)25(27)23
InchiKey:	OGWXZHRXYRVPPS-UHFFFAOYSA-N
Formula:	C27H53NO4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(CCC)NC(=O)OCC(C)C
Mol. weight [g/mol]:	455.72

Physical Properties

Property code	Value	Unit	Source
hf	-1223.66	kJ/mol	Cheméo Relay (1.0)
hfus	69.31	kJ/mol	Joback Method
hvap	129.66	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.68		Cheméo Relay (1.0)
logp	7.952		Crippen Method
mcvol	416.150	ml/mol	McGowan Method
tb	659.24	K	Cheméo Relay (1.0)
tf	321.91	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1475.88	J/mol×K	1019.03	Joback Method
cpg	1497.06	J/mol×K	1059.96	Joback Method
cpg	1516.13	J/mol×K	1100.89	Joback Method
cpg	1533.17	J/mol×K	1141.82	Joback Method
cpg	1548.25	J/mol×K	1182.75	Joback Method
cpg	1561.46	J/mol×K	1223.68	Joback Method
cpg	1572.87	J/mol×K	1264.62	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320725&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/58-372-5/L-Norvaline-N-isobutoxycarbonyl-heptadecyl-ester.pdf>

Generated by Cheméo on 2026-07-22 20:18:40.307011928 +0000 UTC m=+262616.148897347.

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