

L-Norvaline, N-isobutoxycarbonyl-, dodecyl ester

Inchi:	InChI=1S/C22H43NO4/c1-5-7-8-9-10-11-12-13-14-15-17-26-21(24)20(16-6-2)23-22(25)2
InchiKey:	NEXRNOCUCGOTJA-UHFFFAOYSA-N
Formula:	C22H43NO4
SMILES:	CCCCCCCCCCCCOC(=O)C(CCC)NC(=O)OCC(C)C
Mol. weight [g/mol]:	385.59

Physical Properties

Property code	Value	Unit	Source
hf	-1124.87	kJ/mol	Cheméo Relay (1.0)
hfus	56.36	kJ/mol	Joback Method
hvap	110.20	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.10		Cheméo Relay (1.0)
logp	6.001		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
rinpol	2271.00		NIST Webbook
tb	625.41	K	Cheméo Relay (1.0)
tf	304.93	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1158.20	J/mol×K	904.63	Joback Method
cpg	1176.86	J/mol×K	938.47	Joback Method
cpg	1194.17	J/mol×K	972.31	Joback Method
cpg	1210.14	J/mol×K	1006.15	Joback Method
cpg	1224.81	J/mol×K	1039.99	Joback Method
cpg	1238.20	J/mol×K	1073.83	Joback Method
cpg	1250.35	J/mol×K	1107.67	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320721&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>

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

Cheméo Relay (1.0):

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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