

L-Norvaline, N-allyloxycarbonyl-, ethyl ester

Inchi:	InChI=1S/C11H19NO4/c1-4-7-9(10(13)15-6-3)12-11(14)16-8-5-2/h5,9H,2,4,6-8H2,1,3H3
InchiKey:	WQPPQGMDMDHDOW-UHFFFAOYSA-N
Formula:	C11H19NO4
SMILES:	C=CCOC(=O)NC(CCC)C(=O)OCC
Mol. weight [g/mol]:	229.28

Physical Properties

Property code	Value	Unit	Source
hfus	30.12	kJ/mol	Joback Method
logp	1.630		Crippen Method
mcvol	186.410	ml/mol	McGowan Method
rinpol	1467.00		NIST Webbook
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tb	543.31	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.91	J/mol×K	650.07	Joback Method
cpg	510.43	J/mol×K	681.13	Joback Method
cpg	523.27	J/mol×K	712.19	Joback Method
cpg	535.44	J/mol×K	743.24	Joback Method
cpg	546.95	J/mol×K	774.30	Joback Method
cpg	557.79	J/mol×K	805.36	Joback Method
cpg	567.96	J/mol×K	836.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320744&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/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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