

L-Valine, N-(3-methylbut-2-enoyl)-, nonyl ester

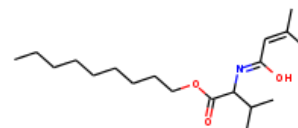
InChI: InChI=1S/C19H35NO3/c1-6-7-8-9-10-11-12-13-23-19(22)18(16(4)5)20-17(21)14-15(2)3/h14,16,18H,6-13H2,1-5H3,(H,20,21)

InChI Key: UATMBZVQRUPTHJ-UHFFFAOYSA-N

Formula: C19H35NO3

SMILES: CCCCCCCCCOC(=O)C(N=C(O)C=C(C)C)C(C)C

Molecular Weight: 325.49



Physical Properties

Property	Value	Unit	Source
$\Delta_f H^\circ_{\text{gas}}$	-663.22	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	86.38	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	5.23		Crippen Method
P_c	1164.04	kPa	Joback Method
T_{boil}	882.31	K	Joback Method
T_c	1082.04	K	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H35NO3/c1-6-7-8-9-10-11-12-13-23-19\(2\)18\(16\(4\)5\)20-17\(21\)14-15\(2\)3/h14,16,18H,6-13H2,1-5H3,\(H,20,21\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H35NO3/c1-6-7-8-9-10-11-12-13-23-19(2)18(16(4)5)20-17(21)14-15(2)3/h14,16,18H,6-13H2,1-5H3,(H,20,21))

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\Delta_f H^\circ_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

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