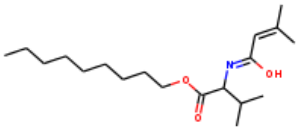
L-Valine, N-(3-methylbut-2-enoyl)-, nonyl ester

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
$\Delta_f H°_{gas}$	-663.22	kJ/mol	Joback Method
$\Delta_{vap} H°$	86.38	kJ/mol	Joback Method
$logP_{oct/wat}$	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(22)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/ci990307l

Legend

$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
$logP_{oct/wat}$: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
T_{boil}: Normal Boiling Point Temperature (K).

T_c: Critical Temperature (K).