

L-norvaline, n-methoxycarbonyl-, hexadecyl ester

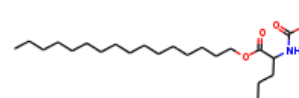
InChI: InChI=1S/C23H45NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-20-28-22(25)21(19-5-2)24-23(26)27-3/h21H,4-20H2,1-3H3,(H,24,26)

InChI Key: YHXGOCXVVBTHQS-UHFFFAOYSA-N

Formula: C₂₃H₄₅NO₄

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(CCC)NC(=O)OC

Molecular Weight: 399.61



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-238.11	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-959.46	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	62.48	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	91.15	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	6.54		Crippen Method
P_c	911.08	kPa	Joback Method
T_{boil}	927.95	K	Joback Method
T_c	1137.94	K	Joback Method
T_{fus}	530.95	K	Joback Method
V_c	1.401	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1220.46	J/mol×K	927.95	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H45NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-20-28-22\(25\)21\(19-5-2\)24-23\(26\)27-3/h21H,4-20H2,1-3H3,\(H,24,26\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H45NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-20-28-22(25)21(19-5-2)24-23(26)27-3/h21H,4-20H2,1-3H3,(H,24,26))

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

Legend

$C_{p, gas}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

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

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

$\Delta_{vap} H^\circ$: 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).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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