DL-Alanine, N-methyl-N-(byt-2-yn-1-yloxycarbonyl)-, tridecyl ester

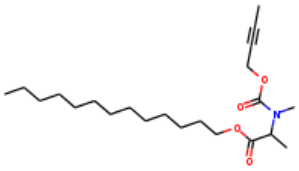
InChI: InChI=1S/C22H39NO4/c1-5-7-9-10-11-12-13-14-15-16-17-19-26-21(24)20(3)23(4)22(25)27-18-8-6-2/h20H,5,7,9-19H2,1-4H3

InChI Key: TZBNODJZOIFGFD-UHFFFAOYSA-N

Formula: C22H39NO4

SMILES: CC#CCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCCC

Molecular Weight: 381.55



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-22.34	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-652.46	kJ/mol	Joback Method
$\Delta_{fus} H°$	60.93	kJ/mol	Joback Method
$\Delta_{vap} H°$	86.68	kJ/mol	Joback Method
$logP_{oct/wat}$	5.32		Crippen Method
P_c	1059.64	kPa	Joback Method
T_{boil}	876.34	K	Joback Method
T_c	1074.36	K	Joback Method
T_{fus}	605.59	K	Joback Method
V_c	1.29	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1085.00	J/mol×K	876.34	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C22H39NO4/c1-5-7-9-10-11-12-13-14-15-16-17-19-26-21(24)20(3)23(4)22(25)27-18-8-6-2/h20H,5,7,9-19H2,1-4H3

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*$P_{oct/wat}$**: 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 (m^3/kg-mol).