

DL-Alanine, N-methyl-N-(but-2-yn-1-yloxy-carbonyl)-, propyl ester

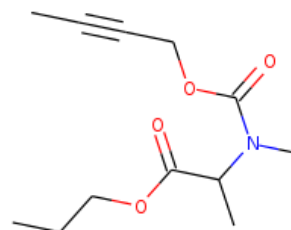
InChI: InChI=1S/C12H19NO4/c1-5-7-9-17-12(15)13(4)10(3)11(14)16-8-6-2/h10H,6,8-9H2,1-4H3

InChI Key: AMSJCALWSRWSFA-UHFFFAOYSA-N

Formula: C₁₂H₁₉NO₄

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

Molecular Weight: 241.28



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-106.54	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-446.06	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	35.03	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	64.42	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.42		Crippen Method
P_c	2241.88	kPa	Joback Method
T_{boil}	647.54	K	Joback Method
T_c	843.92	K	Joback Method
T_{fus}	492.89	K	Joback Method
V_c	0.73	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	513.01	J/mol×K	647.54	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H19NO4/c1-5-7-9-17-12\(15\)13\(4\)10\(3\)11\(14\)16-8-6-2/h10H,6,8-9H2,1-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H19NO4/c1-5-7-9-17-12(15)13(4)10(3)11(14)16-8-6-2/h10H,6,8-9H2,1-4H3)

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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