

# Glycine, N-methyl-n-butoxycarbonyl-, isobutyl ester

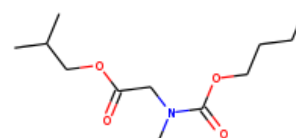
**InChI:** InChI=1S/C12H23NO4/c1-5-6-7-16-12(15)13(4)8-11(14)17-9-10(2)3/h10H,5-9H2,1-4H3

**InChI Key:** SVMHROZKNGYSEX-UHFFFAOYSA-N

**Formula:** C12H23NO4

**SMILES:** CCCCOC(=O)N(C)CC(=O)OCC(C)C

**Molecular Weight:** 245.32



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-309.34	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-718.36	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	31.91	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	62.27	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.05		Crippen Method
$P_c$	1937.24	kPa	Joback Method
$T_{\text{boil}}$	638.54	K	Joback Method
$T_c$	817.39	K	Joback Method
$T_{\text{fus}}$	386.79	K	Joback Method
$V_c$	0.77	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	554.86	J/mol×K	638.54	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H23NO4/c1-5-6-7-16-12\(15\)13\(4\)8-11\(14\)17-9-10\(2\)3/h10H,5-9H2,1-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H23NO4/c1-5-6-7-16-12(15)13(4)8-11(14)17-9-10(2)3/h10H,5-9H2,1-4H3)

**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 (m<sup>3</sup>/kg-mol).

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