

# 4-Butylbenzoic acid, 3-methylbutyl ester

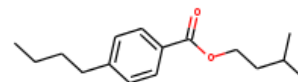
**InChI:** InChI=1S/C16H24O2/c1-4-5-6-14-7-9-15(10-8-14)16(17)18-12-11-13(2)3/h7-10,13H,4-6,11-12H2,1-3H3

**InChI Key:** XFLZSMLNZLATFX-UHFFFAOYSA-N

**Formula:** C16H24O2

**SMILES:** CCCCc1ccc(C(=O)OCCC(C)C)cc1

**Molecular Weight:** 248.36



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-49.74	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-398.59	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	30.11	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	62.92	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.23		Crippen Method
$P_c$	1759.49	kPa	Joback Method
$T_{\text{boil}}$	672.99	K	Joback Method
$T_c$	872.43	K	Joback Method
$T_{\text{fus}}$	366.18	K	Joback Method
$V_c$	0.84	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	600.19	J/mol×K	672.99	Joback Method
$\eta$	0.00	Paxs	672.99	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/C16H24O2/c1-4-5-6-14-7-9-15\(10-8-14\)16\(17\)18-12-11-13\(2\)3/h7-10,13H,4-6,11-12H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H24O2/c1-4-5-6-14-7-9-15(10-8-14)16(17)18-12-11-13(2)3/h7-10,13H,4-6,11-12H2,1-3H3)

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

## Legend

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

$\eta$ : Dynamic viscosity (Pa $\times$ s).

$\Delta_f G^\circ$ : 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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