

# Benzamide, 3-bromo-N-(3-methylbutyl)-

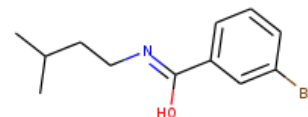
**InChI:** InChI=1S/C12H16BrNO/c1-9(2)6-7-14-12(15)10-4-3-5-11(13)8-10/h3-5,8-9H,6-7H2,1-2H3,(H,14,15)

**InChI Key:** IKJZQBZKPJUEJA-UHFFFAOYSA-N

**Formula:** C12H16BrNO

**SMILES:** CC(C)CCN=C(O)c1cccc(Br)c1

**Molecular Weight:** 270.17



## Physical Properties

Property	Value	Unit	Source
$\Delta_f H^\circ_{\text{gas}}$	-124.70	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	71.36	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.80		Crippen Method
$P_c$	2537.93	kPa	Joback Method
$T_{\text{boil}}$	740.08	K	Joback Method
$T_c$	959.94	K	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/C12H16BrNO/c1-9\(2\)6-7-14-12\(15\)10-4-3-5-11\(13\)8-10/h3-5,8-9H,6-7H2,1-2H3,\(H,14,15\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H16BrNO/c1-9(2)6-7-14-12(15)10-4-3-5-11(13)8-10/h3-5,8-9H,6-7H2,1-2H3,(H,14,15))

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

## Legend

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

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

$\log P_{\text{oct/wat}}$ : Octanol/Water partition coefficient .

$P_c$ : Critical Pressure (kPa).

$T_{\text{boil}}$ : Normal Boiling Point Temperature (K).

$T_c$ : Critical Temperature (K).

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