

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

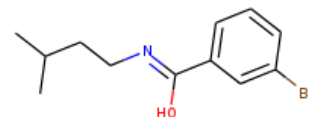
InChI: InChI=1S/C12H16BrNO/c1-9(2)6-7-14-12(15)10-4-3-5-11(13)8-10/h3-5,8-9H,6-7H2,1-2H3,(H,14,15)

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
$\log P_{\text{oct/wat}}$	3.800		Crippen Method
P_c	2537.93	kPa	Joback Method
T_{boil}	740.08	K	Joback Method
T_c	959.94	K	Joback Method

Sources

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_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

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