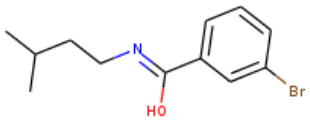
Benzamide, 3-bromo-N-(3-methylbutyl)-

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
$\Delta_f H°_{gas}$	-124.70	kJ/mol	Joback Method
$\Delta_{vap} H°$	71.36	kJ/mol	Joback Method
$logP_{oct/wat}$	3.80		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)
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{vap} H°$: 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).