

2-Bromo-2-methylpropane Structure - C₄H₉Br - Over 100 million chemical compounds | Mol-Instincts

Chemical Structure Description

A chemical structure of a molecule includes the arrangement of atoms and the chemical bonds that hold the atoms together. The 2-Bromo-2-methylpropane molecule contains a total of 13 bond(s) There are 4 non-H bond(s). Images of the chemical structure of 2-Bromo-2-methylpropane are given below:

The 2D chemical structure image of 2-Bromo-2-methylpropane is also called skeletal formula, which is the standard notation for organic molecules.

- Lower Flammability Limit Volume Percent
- Upper Flammability Limit Temperature
- Upper Flammability Limit Volume Percent
- Liquid Density
- Heat of Vaporization at 298.15K
- Heat of Vaporization at Normal Boiling Point

- Heat Capacity of Ideal Gas
- Heat Capacity of Liquid
- Heat of Vaporization

- Liquid Density
- Surface Tension
- Thermal Conductivity of Liquid

- Thermal Conductivity of Gas
- Vapor Pressure of Liquid
- Viscosity of Liquid

- Viscosity of Gas
- Second Virial Coefficient

- LogP (Octanol-Water Partition Coefficient)
- LogS (Water Solubility)
- Number of Acceptor Atoms for H-bonds
- Number of Donor Atoms for H-bonds

- Ghose-Crippen Molar Refractivity
- Ghose-Crippen Octanol-Water Partition Coefficient (logP)
- Moriguchi Octanol-Water Partition Coefficient (logP)
- Lipinski Alert Index

- Drug-likeness
- Activity Score for GPCR Ligands
- Activity Score for Ion Channel Modulators
- Activity Score for Kinase Inhibitors

- Activity Score for Nuclear Receptor Ligands

- IR spectra

- NMR spectra

- VCD spectra

- 3D Visualization, Animation & Analysis
 - Interactive Optimized Structure
 - Measurement of Bond Length and Angle
 - Normal Mode Frequency Analysis with Animation
 - Molecular Orbital (HOMO & LUMO) Visualization

- quantum Chemical Computation Data (20 sets)

- Molecular Descriptors
 - 24 Categories
 - Total of 2,004 Sets

Additional Information for Identifying 2-Bromo-2-methylpropane Molecule

• SMILES (Simplified Molecular-Input Line-Entry System) string of 2-Bromo-2-methylpropane

The SMILES string of 2-Bromo-2-methylpropane is CC(C)(C)Br, which can be imported by most molecule editors for conversion back into two-dimensional drawings or three-dimensional models of the 2-Bromo-2-methylpropane.

• Structure Data File (SDF/MOL File) of 2-Bromo-2-methylpropane

The structure data file (SDF/MOL File) of 2-Bromo-2-methylpropane is available for download in the SDF page of 2-Bromo-2-methylpropane, which provides the information about the atoms, bonds, connectivity and coordinates of 2-Bromo-2-methylpropane. The 2-

Bromo-2-methylpropane structure data file can be imported to most of the cheminformatics software systems and applications.

• Chemical formula of 2-Bromo-2-methylpropane

The molecular formula of 2-Bromo-2-methylpropane is available in chemical formula page of 2-Bromo-2-methylpropane, which identifies each constituent element by its chemical symbol and indicates the proportionate number of atoms of each element.

• Molecular weight of 2-Bromo-2-methylpropane

The molecular weight of 2-Bromo-2-methylpropane is available in molecular weight page of 2-Bromo-2-methylpropane, which is calculated as the sum of the atomic weights of each constituent element multiplied by the number of atoms of that element in the molecular formula.

• Other names (synonyms) or registry numbers of 2-Bromo-2-methylpropane

The 2-Bromo-2-methylpropane compound may be called differently depending on the various different situations of industrial applications. Below are the list of the other names (synonyms) of 2-Bromo-2-methylpropane including the various registry numbers, if available:

- BBV-34551764
- Z1262252890
- W-105932
- I14-0269
- 2-Bromo-2-methylpropane, purum, $\geq 97.0\%$ (GC)
- A828265
- tert-Butyl bromide, 98%, stabilized 100g
- B0617
- RTR-018130
- MFCD00000125
- ANW-31109
- 5LWO08435U
- 2-Bromo-2-methylpropane, 98%
- 2-bromanyl-2-methyl-propane
- UN 2342 (Related)
- 2-Bromo-2-methyl propane
- 2-bromo-2methyl-propane
- tertiary-butyl bromide
- tert-C4H9Br
- sJPHAbIMUP@
- Butylbromide, tert-
- tert.butyl bromide
- tert.-butylbromide
- tert. butylbromide
- tertbutyl bromide
- tertbutylbromide
- t-butylbromide
- LABOTEST-BB LTBB001549
- 1,1-Dimethylethyl bromide
- 1,1-Dimethylethyl chloride
- 2-Bromo-2-methyl-propane
- tert-butylbromide
- 2-methyl-2-bromopropane
- 1-Bromo-1,1-dimethylethane
- Tertiarybutyl bromide
- 2-Bromoisobutane
- Bromotrimethylmethane
- Propane, 2-bromo-2-methyl-
- Trimethylbromomethane
- T-BUTYL BROMIDE
- 507-19-7
- tert-Butyl bromide

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2-Bromo-2-methylpropane Identification Summary Frequently Asked Questions (FAQs)

What's the chemical formula of 2-Bromo-2-methylpropane? C_4H_9Br How many atoms and what are the elements included the 2-Bromo-2-methylpropane molecule? 14 atom(s) - 9 Hydrogen atom(s), 4 Carbon atom(s) and 1 Bromine atom(s) How many chemical bonds and what kind of bonds are included the 2-Bromo-2-methylpropane structure? 13 bond(s) - 4 non-H bond(s) What's the 2-Bromo-2-methylpropane's molecular weight? 137.01826 g/mol What's the SMILES code of 2-Bromo-2-methylpropane? CC(C)(C)Br What's the InChI string of 2-Bromo-2-methylpropane? InChI=1S/C4H9Br/c1-4(2,3)5/h1-3H3 What's the InChIKey code of 2-Bromo-2-methylpropane? RKSOPLXZQNSWAS-UHFFFAOYSA-N

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