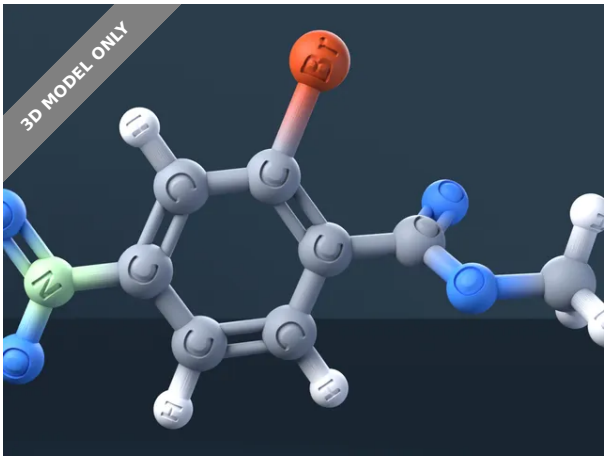

Methyl 2-Bromo-4-nitrobenzoate 3D Molecular Model — CAS 100959-22-6

MolGod Scientific

VIEW IN BROWSER

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Summary

Free educational Methyl 2-Bromo-4-nitrobenzoate model (CAS 100959-22-6), engraved element symbol on every atom.

Learning > Chemistry & Biology

Tags: education teaching stem chemistry stl aromatic classroom molecule engraved molecularmodel ester isomers chemistryeducation aromaticity molgod nitrocompound organohalogen

Methyl 2-Bromo-4-nitrobenzoate (C8H6BrNO4, CAS 100959-22-6) — a free educational 3D molecular model for teachers and students, by MolGod.org. Symbols are engraved into every atom, so students read atoms by symbol, not by colour.

At its heart, Methyl 2-Bromo-4-nitrobenzoate is built around one aromatic 6-membered ring. The model shows 20 bonds: 12 single, 2 double and 6 aromatic, drawn in Kekulé form. A five-minute warm-up: read the symbol on every sphere and write down the totals (8 C + 6 H + 1 Br + 1 N + 4 O = 20 atoms). Functional groups to find on the model: ester group (-COO-),

nitro group (-NO2) and C-Br bond. Topics it supports in class: aromaticity and delocalised electrons, the carbonyl group (C=O), as well as organohalogen compounds and carbon-halogen bonds. Ask students what this molecule has in common with 4-Bromomethyl-3-nitrobenzoic acid (CAS 55715-03-2), then what sets them apart; the molecular formula is shared.

MolGod.org offers this engraved model free to anyone teaching or learning chemistry. Teachers: give each table a model and have students write the formula from the engraved atoms.

Full record and more free models: https://molgod.org/molecule/100959-22-6/?utm_source=printables&utm_medium=referral&utm_campaign=edu-3d-models
Licence & provenance: https://molgod.org/licenses/stl/100959-22-6/
Same file on Wikimedia Commons: https://commons.wikimedia.org/wiki/File:Methyl_2-Bromo-4-nitrobenzoate-3D-molecular-model-engraved-CAS-100959-22-6.stl

A ball-and-stick model of Methyl 2-Bromo-4-nitrobenzoate with each element symbol recessed into its atom sphere, generated by MolGod.org from a PubChem-computed 3D conformer (not an experimental crystal structure); atomic coordinates and connectivity are unchanged. STL mesh: 293,682 triangles, closed (watertight) single solid. Coordinates in ångström (STL stores no unit) — scale the model deliberately in your slicer.

Chemical identity

- CAS Registry Number: 100959-22-6
- Molecular formula: C8H6BrNO4
- Molar mass: 260.04 g/mol (exact mass 258.94802)
- IUPAC name: methyl 2-bromo-4-nitrobenzoate
- MolGod ID: MG_278-907-634-69 (https://molgod.org/id/MG_278-907-634-69)
- PubChem CID: 15833211 (https://pubchem.ncbi.nlm.nih.gov/compound/15833211)
- Wikidata: Q72488771 (https://www.wikidata.org/wiki/Q72488771)
- EC number: 640-134-2
- InChIKey: XYMZAFDNPJLOTP-UHFFFAOYSA-N
- SMILES: COC(=O)C1=C(C=C(C=C1)[N+](=O)[O-])Br

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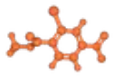
Model files



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