



Office helper



I wish to know about ibuprofen, I want to know its MW, SMIELS, logP

Intentionally misspelled the property 'SMIELS', question identified by the chatbot.



Ibuprofen is a well-known nonsteroidal anti-inflammatory drug (NSAID) used to relieve pain, reduce inflammation, and lower fever. Here are the chemical properties you requested:

- **Molecular Weight (MW):** 206.28 g/mol
- **SMILES (Simplified Molecular Input Line Entry System):**
CC(C)CC1=CC=C(C=C1)C(C)C(=O)O
- **logP (Octanol/Water Partition Coefficient):** 3.07

MW, SMILES, logP accurate, showing the RDKit and PubChem APIs functioning well.

These properties are useful in understanding the behavior of ibuprofen in biological systems, such as its solubility and permeability. If you have any more questions or need further information, feel free to ask!



great, can I get PDB ID from the chemical name?

Web search triggered when search is not supported by our tool planner.



Certainly! The PDB ID for the structure of ibuprofen bound to cyclooxygenase-2 is 4PH9. If you have any more questions about chemical structures or properties, feel free to ask!



Good, help me explore the resolution of the protein?

Resolution accurate, PDB API functioning well.



Certainly! The protein structure you're referring to, with the PDB ID 4PH9, has a resolution of 1.81 Ångströms. This resolution indicates the level of detail at which the protein structure has been determined using X-ray diffraction methods. A resolution of 1.81 Å is considered quite high, allowing for detailed visualization of the protein's atomic arrangement. This particular structure is of ibuprofen bound to cyclooxygenase-2, a protein from *Mus musculus* (house mouse), expressed in *Spodoptera frugiperda* (a species of moth).



great, now I want to know the TPSA and similar molecules of it.

Clarification required
when the question is
ambiguous, as PDB ID
can refer to different
SMILES



To help you with the Topological Polar Surface Area (TPSA) and similar molecules, I would need to know the specific chemical compound you are interested in. Please provide the name or structure of the compound, and I'll do my best to provide the information you need.

Ask me something about a molecule...

