



Office helper



tell me smiles of aspirin

Pubchem working appropriately.



The SMILES (Simplified Molecular Input Line Entry System) representation for aspirin is: CC(=O)OC1=CC=CC=C1C(=O)O. This notation provides a way to describe the structure of the aspirin molecule using a string of text, which is useful for computational chemistry applications.

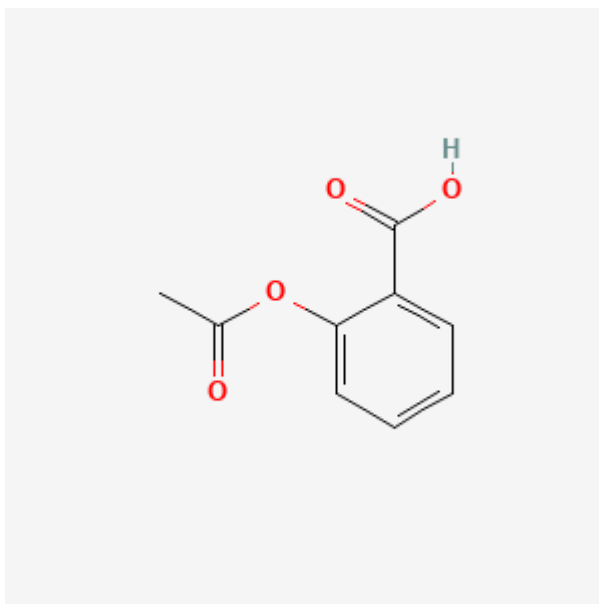


I also want to see the 2d structure

Supports image and text output to improve use experience.



Certainly! Here is the 2D structure of aspirin, a commonly used medication known for its pain-relieving and anti-inflammatory properties:



In addition to the visual representation, the SMILES (Simplified Molecular Input Line Entry System) notation for aspirin is: CC(=O)OC1=CC=CC=C1C(=O)O. This notation provides a way to describe the structure of a chemical compound using a string of text, which is useful for computational purposes.



great, and I want the logP as well.

logP accurate.



Aspirin, known chemically as acetylsalicylic acid, has a logP value of 1.31. The logP value is a measure of the compound's hydrophobicity, indicating how well it partitions between water and octanol. A logP of 1.31 suggests that aspirin is moderately hydrophobic, meaning it has a balanced solubility between water and lipids, which is useful for its absorption in the body.

If you need more information or have further questions about aspirin, feel free to ask!



well done, now let's get some patents and web information about it.



Here is some patent and web information related to aspirin and its applications:

Patents

1. Aspirin-induced lipid mediator

- **Inventor:** Charles Serhan
- **Patent Status:**
 - US: Active
 - EP: Active
 - CN: Active
- [Link to Patent](#)

2. Compositions comprising lecithin oils and NSAIDs for protecting the gastrointestinal tract and providing enhanced therapeutic activity

- **Inventor:** Lenard M. Lichtenberger
- **Patent Status:**
 - US: Active
- [Link to Patent](#)

3. Oral dosage forms including an antiplatelet agent and an acid inhibitor

- **Inventor:** Mark A. Goldsmith
- **Patent Status:**

- US: Active
- EP: Active
- CN: Active
- [Link to Patent](#)

Web Information

Aspirin, chemically known as acetylsalicylic acid (C₉H₈O₄), is a widely used medication due to its analgesic, antipyretic, and anti-inflammatory properties. It works by inhibiting the cyclooxygenase enzyme, thus reducing the production of prostaglandins and thromboxanes, which are involved in pain, inflammation, and blood clotting.

The synthesis of aspirin is typically performed by acetylating salicylic acid with acetic anhydride, a process often catalyzed by phosphoric acid. This synthesis is a staple in educational settings, showcasing fundamental organic chemistry techniques. Additionally, aspirin's molecular and crystal structures have been extensively studied, underscoring its importance in both medicinal and industrial contexts.

These patents and information highlight the ongoing research and development in the field of aspirin and its applications, reflecting its significance in healthcare and pharmaceutical industries.

Ask me something about a molecule...

