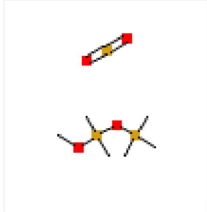





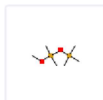


COMPOUND SUMMARY

# Simethicone

PubChem CID	6433516
Structure	<div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;">  <p>2D</p> </div> <div style="text-align: center;">  <p>3D</p> </div> </div>
Chemical Safety	<div style="display: flex; justify-content: center; gap: 20px;"> <div style="text-align: center;">  <p>Flammable</p> </div> <div style="text-align: center;">  <p>Irritant</p> </div> </div> <p style="text-align: center; color: #0070C0;"> <a href="#">Laboratory Chemical Safety Summary (LCSS) Datasheet</a> </p>
Molecular Formula	$C_6H_{18}O_4Si_3$
Synonyms	<p>Simethicone        8050-81-5        dioxosilane;methoxy-dimethyl-trimethylsilyloxysilane        SIMETICONE        SCHEMBL339371</p> <p style="text-align: center; border: 1px solid #ccc; padding: 2px 5px; display: inline-block;">View More...</p>
Molecular Weight	<p>238.46 g/mol</p> <p style="font-size: small; color: #666;"><i>Computed by PubChem 2.1 (PubChem release 2021.05.07)</i></p>
Parent Compound	<div style="display: flex; align-items: center;"> <div style="margin-right: 10px;">  </div> <p style="color: #0070C0;"> <a href="#">CID 87479 (Disiloxane, methoxypentamethyl-)</a> </p> </div>
Component Compounds	<div style="display: flex; align-items: center;"> <div style="margin-right: 10px;">  </div> <p style="color: #0070C0;"> <a href="#">CID 24261 (Silicon Dioxide)</a> </p> </div>



CID 87479 (Disiloxane, methoxypentamethyl-)

## Dates

Create: 2006-04-28  
Modify: 2023-12-10

## Description

Simethicone is a **silicon** based surfactant that decreases the surface tension of gastrointestinal gas bubbles to facilitate their elimination. It has a favourable safety profile as it is not systemically absorbed. Simethicone has been in use since the 1940s but was granted FDA approval in 1952.

▶ [DrugBank](#)

Simethicone is a mixture of polydimethylsiloxanes with antifoaming and anti-bloating effects. Simethicone reduces the surface tension of gas bubbles causing them to coalesce into larger bubbles that can be passed more easily by belching or flatulence.

▶ [NCI Thesaurus \(NCIt\)](#)

A poly(dimethylsiloxane) which is a polymer of 200-350 units of dimethylsiloxane, along with added silica gel. It is used as an antiflatulent, surfactant, and ointment base.

▶ [Medical Subject Headings \(MeSH\)](#)

## Contents

### Title and Summary

### 1 Structures



### 2 Names and Identifiers



### 3 Chemical and Physical Properties



### 4 Related Records



### 5 Chemical Vendors

### 6 Drug and Medication Information



### 7 Food Additives and Ingredients



### 8 Pharmacology and Biochemistry



### 9 Use and Manufacturing



10 Safety and Hazards



11 Toxicity



12 Associated Disorders and Diseases

13 Literature



14 Patents



15 Interactions and Pathways



16 Classification

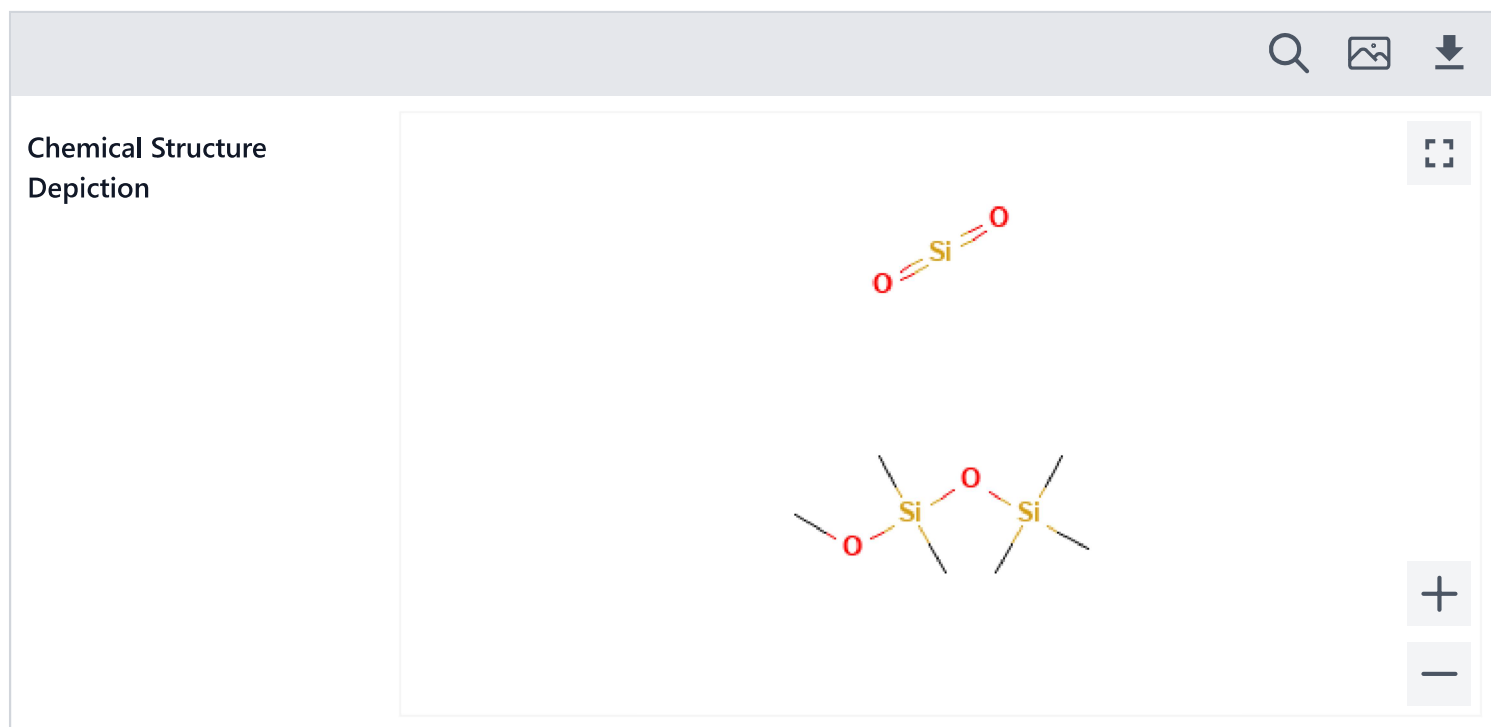


17 Information Sources

## 1 Structures



### 1.1 2D Structure



► PubChem

### 1.2 3D Conformer



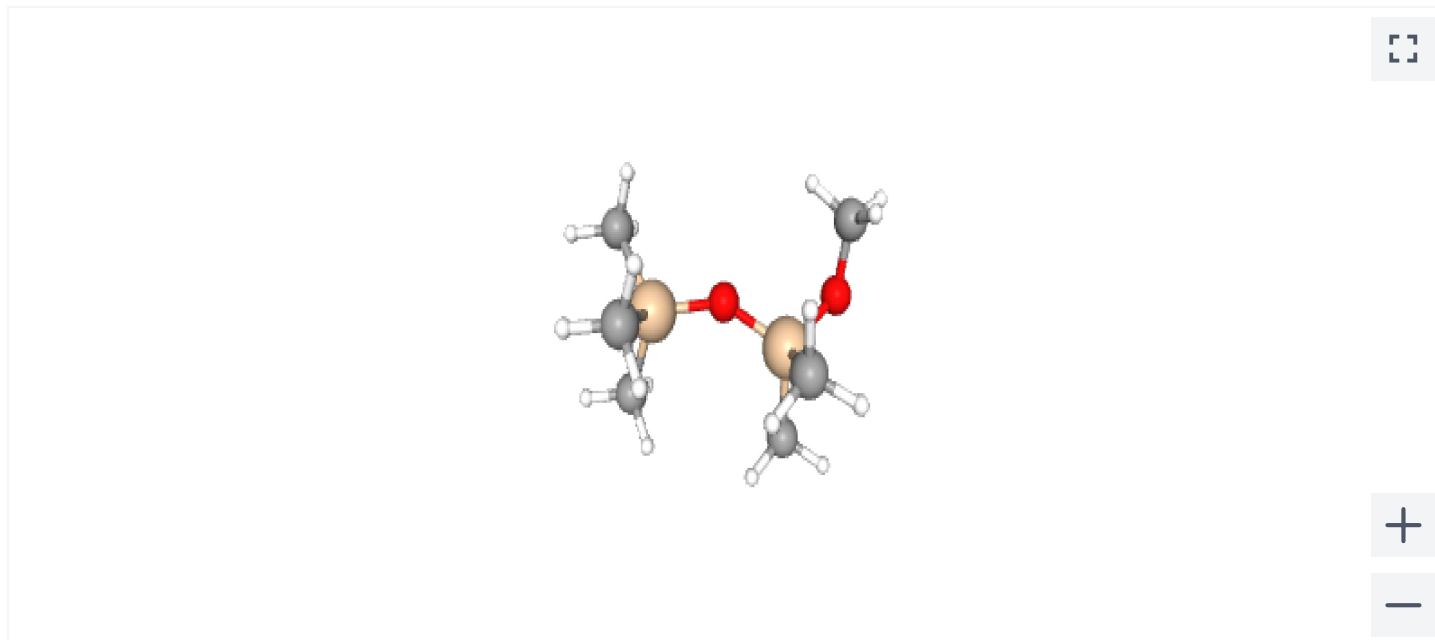
3D Conformer of Parent



### Interactive Chemical Structure Model

Ball and Stick  Sticks  Wire-Frame  Space-Filling

Show Hydrogens  Animate



<< First < Previous Conformer 1 of 4 Next > Last >>

▶ [PubChem](#)

## 2 Names and Identifiers 🔍 ↗

### 2.1 Computed Descriptors 🔍 ↗

#### 2.1.1 IUPAC Name 🔍 ↗

dioxosilane;methoxy-dimethyl-trimethylsilyloxysilane

*Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)*

▶ [PubChem](#)

#### 2.1.2 InChI 🔍 ↗

InChI=1S/C6H18O2Si2.O2Si/c1-7-10(5,6)8-9(2,3)4;1-3-2/h1-6H3;

*Computed by InChI 1.0.6 (PubChem release 2021.05.07)*

▶ [PubChem](#)

## 2.1.3 InChIKey



AMTWCFIKVBGOD-UHFFFAOYSA-N

*Computed by InChI 1.0.6 (PubChem release 2021.05.07)*

▶ [PubChem](#)

## 2.1.4 Canonical SMILES



CO[Si](C)(C)O[Si](C)(C)C.O=[Si]=O

*Computed by OEChem 2.3.0 (PubChem release 2021.05.07)*

▶ [PubChem](#)

## 2.2 Molecular Formula



$C_6H_{18}O_4Si_3$

*Computed by PubChem 2.1 (PubChem release 2021.05.07)*

▶ [PubChem](#)

## 2.3 Other Identifiers



### 2.3.1 CAS



8050-81-5

▶ [DrugBank](#); [European Chemicals Agency \(ECHA\)](#); [Hazardous Substances Data Bank \(HSDB\)](#)

### 2.3.2 European Community (EC) Number



617-098-1

▶ [European Chemicals Agency \(ECHA\)](#)

933-297-9