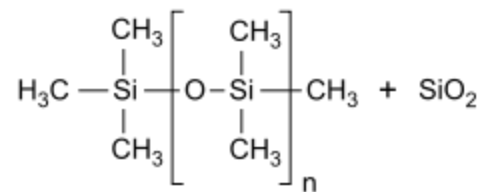# Case 2:

Simethicone

Group 1 Specified Substance
Multiple Substance Ingredient
Properties
Amounts
Reference Documents
Decision Tree
In-Place entity Searching

Premise:

Well-populated System

Dimethicone is already registered
Silicon dioxide is already registered

Home   **Search**   **Download**   **Register**   **Admin**

Register New:

Substance	Product

◁   ▷

Home   **Search**   **Download**   **Register**   **Admin**

Register New:

Substance	Product

Single Substance	Mixture Substance	Specified Substance	Not Sure

GINAS

Home   **Search**   **Download**   **Register**   **Admin**

Register New:

Substance	Product

Single Substance	Mixture Substance	Specified Substance	Not Sure

Is there more than one covalent moiety in this material?	Yes	No	?

Is this a stereochemical mixture only?	Yes	No	?

Do these entities form a stoichiometric or crystallizable ensemble?	Yes	No	?

Were all entities intentionally isolated from the same synthetic process?	Yes	No	?

Were all entities isolated from the same source material?	Yes	No	?

Do these entities form a single ingredient?	Yes	No	?

Register New:

| Substance | Product |

| Single Substance | Mixture Substance | Specified Substance | Not Sure |

(?) **Group 1** — Mixtures of single substances, and specific physical forms of substances.

(?) **Group 2** — Limited production method information.

(?) **Group 3** — Material at a specific grade.

(?) **Group 4** — Detailed production and manufacturing information.

Peryeat logout

Home   Search   Download   **Register**   Admin

Name:

Simethicone

Language: English +

Domain: Drug +

Name Type: Common Name ▼

Public Domain: ☑

Official Name

Source:

Systematic Name

Source: Code   **Source Doc:**   **Source Date:**

SOURCE   Common Name   04/11/2012 +

◀   Skip   ▶

Home   **Search**   **Download**   **Register**   **Admin**

Name:

Simethicone

Language: English ➕

Domain: Drug ➕

Name Type: Official Name ▾

Public Domain: ☑

Naming Org: USAN ▾   **Deprecated:** ☐   **Deprecated Date:** N/A 📅 ➕

Official Jurisdiction: US ➕

Source:

Source:	**Source-URL:**	**Source Doc:**	**Source Date:**
Martindale ▾	http://example.com	DOC_123.pdf ⬆	04/18/2012 📅 ➕

◀   Skip   ▶

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Home   **Search**   **Download**   **Register**   **Admin**

Constituents:

Add New

Choose

◄   ►

| Names | Amounts | Properties | Documents |

Name:	Type:	Language:	Domain:	Preferred:	
Simethicone	Official	English	Drug	☑	❌
سيميتيكون	Official	Arabic	Drug	☐	❌

◄   **Register**   ►

Select Substance as Constituent

Substances matching **"Dimethicone"**
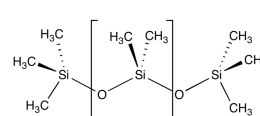
Dimethicone

Search

UNII_92RU3N3Y1O
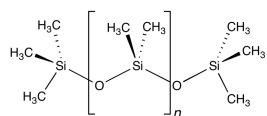
Dimethicone

UNII_RO266O364U
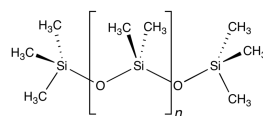
Dimethicone 100

UNII_RGS4T2AS00

Dimethicone 200

15 Results

Cancel   **Select**

GINAS

Home   **Search**   **Download**   **Register**   **Admin**

Constituents:

UNII_92RU3N3Y1O
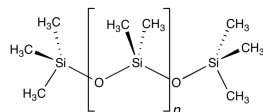
Dimethicone

Constituent ▾

Add New

Choose

Names	Amounts	Properties	Documents

Name:	*Type:*	*Language:*	*Domain:*	*Preferred:*	
Simethicone	Official	English	Drug	☑	❌
سيميتيكون	Official	Arabic	Drug	☐	❌

Register

Select Substance as Constituent

Substances matching **"Silicon Dioxide"**

Silicon Dioxide

Search

UNII_ETJ7Z6XBU4

SiO_2

Silicon Dioxide

1 Result

Cancel

Select
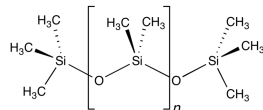
🔍

Constituents:

UNII_92RU3N3Y1O

UNII_ETJ7Z6XBU4

Add New

SiO_2

Choose

Dimethicone

Silicon Dioxide

Constituent ▼   **Constituent** ▼

Names   Amounts   Properties   Documents

Mol Ratio ▼   *Avg:*   *Low:*   *High:*

Entered   UNII-92RU3N3Y1O :

Normalized   UNII-ETJ7Z6XBU4 :

Register
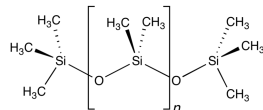
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Home   **Search**   **Download**   **Register**   **Admin**

Constituents:

UNII_92RU3N3Y1O

UNII_ETJ7Z6XBU4

Add New

SiO_2

Choose

Dimethicone

Silicon Dioxide

Constituent ▼

Constituent ▼

Names	Amounts	Properties	Documents

Mol Ratio ▼	*Avg:*	*Low:*	*High:*
Weight Percent			
Entered	Mol Ratio		
Normalized	**Volume Ratio**		

Register

GINAS

Home **Search** **Download** **Register** **Admin**

Constituents:

UNII_92RU3N3Y1O

Dimethicone

[Constituent ▼]

UNII_ETJ7Z6XBU4

SiO$_2$
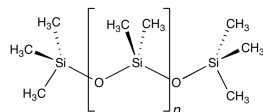
Silicon Dioxide

[Constituent ▼]

Add New

[Choose]

| Names | **Amounts** | Properties | Documents |

Weight Percent ▼

	Avg:	*Low:*	*High:*
Entered			
UNII-92RU3N3Y1O :	95	90.5	99.0
Normalized			
UNII-ETJ7Z6XBU4 :	5.5	4.0	7.0

Register

Constituents:

UNII_92RU3N3Y1O	UNII_ETJ7Z6XBU4	Add New
	SiO$_2$	**Choose**
Dimethicone	**Silicon Dioxide**	

◀ ▶

Constituent ▼   **Constituent** ▼

| Names | **Amounts** | Properties | Documents |

Weight Percent ▼

	Avg:	*Low:*	*High:*
Entered			
Normalized			
UNII-92RU3N3Y1O :	17.27	16.45	18.00
UNII-ETJ7Z6XBU4 :	1.00	0.73	1.27

Register

◀ ▶

GINAS

Home   **Search**   **Download**   **Register**   **Admin**

Constituents:

UNII_92RU3N3Y1O

Dimethicone

Constituent ▼

UNII_ETJ7Z6XBU4

SiO_2

Silicon Dioxide

Constituent ▼

Add New

Choose

| Names | Amounts | Properties | Documents |

Property: *Value:*   *Defining:*

➕

Register

Property: Property ▼

Notes:

Cancel   Done

Property:

Physical Form ▼

Physical Form

Melting Point

Boiling Point

Density

Notes:

Cancel

Property: Physical Form ▼

Value: ▼

Notes:

Cancel   Done

Property: Physical Form ▼

Value: ▼

| Solid |
| Liquid |
| Gas |

Notes:

Cancel

Property: Physical Form ▼

Value: Liquid ▼

Notes:

Cancel   Done

Home   **Search**   **Download**   **Register**   **Admin**
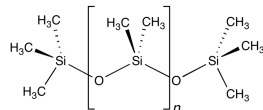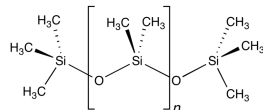
Constituents:

UNII_92RU3N3Y1O

Dimethicone

Constituent ▼

UNII_ETJ7Z6XBU4

SiO_2

Silicon Dioxide

Constituent ▼

Add New

Choose

| Names | Amounts | Properties | Documents |

Property: *Value:*   *Defining:*

Physical Form   **Liquid**   ☑ ✖ ➕

Register

Property: Property ▼

Notes:

Cancel   Done

Property:

Property ▼

Physical Form

Melting Point

Boiling Point

Density

Notes:

Cancel

Property: Density ▼

	Avg:	Low:	High:
Value:			g/mL

Notes:

Cancel   Done

Property: Density ▼

	Avg:	*Low:*	*High:*	
Value:	0.99	0.98	1.00	*g/mL*

Notes: Measured at 20 C.

Cancel   Done

GINAS

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Constituents:

UNII_92RU3N3Y1O

Dimethicone

▼ **Constituent**

UNII_ETJ7Z6XBU4

SiO_2

Silicon Dioxide

▼ **Constituent**

Add New

Choose

| Names | Amounts | Properties | Documents |

Property: | *Value:* | *Defining:*

Physical Form | **Liquid** | ☑ | ❌

Specific Gravity | **0.99** [0.98 - 1.00] | ☐ | ❌ | ➕

Register

Home   **Search**   **Download**   **Register**   **Admin**
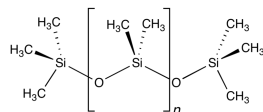
Constituents:

UNII_92RU3N3Y1O   UNII_ETJ7Z6XBU4   **Add New**

SiO_2 **Choose**

Dimethicone   **Silicon Dioxide**

Constituent ▼   **Constituent** ▼

| Names | Amounts | Properties | Documents |

Type: *Sub Type:*   *Document:*   *Date:*

Spectra ▼   **NMR-COSY**   nmr_cozy.pdf   📤   04/18/2012   📅   ❌   ➕

Register