

## SML6 の予測精度を向上させるデータ・ベースの利用

<https://pubchem.ncbi.nlm.nih.gov/>

<https://www.molinspiration.com/cgi/properties>



PubChem

molinspiration  
cheminformatics

2023\_11\_11

2023\_11\_26 改訂版

Table\_03 : 移行モデルPiringer式とWelle式による拡散係数Dpの違い Dp値は20℃における値です。

Migrant	CAS.No	Moleqular Weight	Molecular Volume	Dp Welle	Dp Piringer Upper	Dp_Piringer Realistic
アセトアルデヒド	75-07-0	44.05				
ホルムアルデヒド	50-00-0	30.03				
トルエン	108-88-3	92.14				
ベンゼン	71-43-2	78.11				
ビスヒドロキシエチル テレフタル酸	959-36-2					
ジエチレングリコール	111-46-6	106.12				

テクニカル・ノート SML6.6\_No.14 ではより実測値に近い溶出量が得られる移行モデル\_Welle式 を紹介しています。

Welle法は拡散係数と予測するために移行物質(Migrant) のモル体積を使います。

Molecular Volumeを求めるには

**PubChem+Molinspiration** の合わせ技を使うことが一番の近道です。

molinspiration

オリジナルスマイル C1=CC=C2C(=C1)C(=CC=C2C3=NC4=CC=CC=C4O3)C5=NC6=CC=CC=C6O5  
 ミススマイル C1=CC=C2C(=C1)C(=CC=C2C3=NC4=CC=CC=C4O3)C5=NC6=CC=CC=C6O5  
 2,2'-(1,4-ナフタレンジイル)ビスベンゾオキサゾール

Molinspiration\_erseviz\_engine v2021.10

title	6.47
TPSA	52.00
rotass	28
RT	302.28
nOH	4
nOHmax	0
rotations	1
erorb	2
valmax	312.06

Get\_data\_as\_text (for copy / paste).  
 Get\_3D\_model: BETA

これは、あなたのサイトで今利用可能な1000のうち153,134,7のリクエストでした。Molinspirationのアカウントを  
 使用すると、インターネット上で迅速な検索サービスを提供することができます。  
 コメントや質問? 私たちの[FAQ](#)を見て、フィードバックを提供するか、電子メールで私達に連絡することを躊躇しないでください。

<https://pubchem.ncbi.nlm.nih.gov/>

<https://www.molinspiration.com/cgi/properties>

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SEARCH FOR

111-46-6

Treating this as a text search.

BEST MATCH

 DIETHYLENE GLYCOL; 111-46-6; 2,2'-Oxydiethanol; Diglycol; 2,2'-Oxybisethanol; 2-(2-Hydroxyethoxy)ethanol; Diethylenglykol; Digol; ...

Compound CID: 8117  
MF: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub> MW: 106.12g/mol  
IUPAC Name: 2-(2-hydroxyethoxy)ethanol  
Isomeric SMILES: C(COCCO)O  
InChIKey: MTHSVFCYNBDYFN-UHFFFAOYSA-N  
InChI: InChI=1S/C4H10O3/c5-1-3-7-4-2-6/h5-6H,1-4H2  
Create Date: 2005-03-26

[Summary](#) [Similar Structures Search](#) [Related Records](#)

## COMPOUND SUMMARY

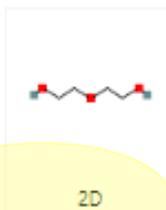
# Diethylene glycol

See also: [Polyester-5 \(tg-38\)](#) (monomer of); [Polyester-5 \(TG-55\)](#) (monomer of); [Polyester-5 \(TG-48\)](#) (monomer of) ... [View More ...](#)

PubChem CID

8117

Structure



Chemical Safety



Irritant

[Laboratory Chemical Safety Summary \(LCSS\) Datasheet](#)

Cite

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Diethylene glycol | C<sub>4</sub>H<sub>10</sub>O<sub>3</sub> | Cl x +

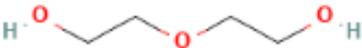
pubchem.ncbi.nlm.nih.gov/compound/8117#section=2D-Structure

PubChem Diethylene glycol (Compound)

### 1.1 2D Structure

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Chemical Structure Depiction



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<https://www.molinspiration.com/cgi/properties>を使うには

Welle法を使うにはMigrantの分子量(g/mol)ではなく、モル体積が必要です。

Migrantの化学式をSIMLES表示にして、MolinspirationのSMILES表記を入力すればモル体積が判明します。(これは2023\_07までは可能でした)

Molinspirationはスロバキアの大学のベンチャーですが、Molinspirationデータベースの評価が得られた時点で2023\_10月からSMILES表記でデータベースを探索することができなくなりました。Molinspirationと個別に契約すればSMILES入力は可能です。

ただしMolinspirationの入力欄に化学式を2Dで描写(書き込み)すれば、分子特性が表示されモル体積情報が得られます。[化学式を入力画面で2Dで描写するか](#)、あるいは[SDF file を貼付ける](#) と分子特性情報が得られます。

~~(8～17ページに入力欄に[化学式を2Dで書き込みする操作法を紹介](#)します。)~~

18～28ページに入力欄に [SDF file を貼付ける操作法を紹介](#)します。

注：ChemDrawの操作に慣れていたとしても、SDFファイルのコピペ操作が簡単です。

2023\_11\_11

2023\_11\_26 追加編集

操作法の事例としてジエチレングリコール（CAS.No.111-46-6）で説明しています。  
左側がPubChem画面、右がmolinspirationです。

The image shows two browser windows. The left window is PubChem, displaying the 2D structure of Diethylene glycol (CAS 111-46-6) and a table of contents. The right window is molinspiration, showing the 'Calculation of Molecular Properties and Bioactivity Score' interface. The molinspiration interface includes a chemical editor toolbar, a central workspace with a yellow circle, and buttons for 'Calculate Properties', 'Predict Bioactivity', and 'Galaxy 3D Generator'.

PubChemでジエチレングリコールの"2D\_structure"を探索します。  
次にmolinspirationの入力欄に 2D\_structureを1つ1つ書き込みます。

本ページから18ページにスキップしてお読みください。

Diethylene glycol | C<sub>4</sub>H<sub>10</sub>O<sub>3</sub> | C x +

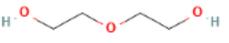
pubchem.ncbi.nlm.nih.gov/compound/8117#section=2D-Structure

PubChem Diethylene glycol (Compound)

### 1.1 2D Structure

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1.2 3D Conformer

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Calculation of molecular propert x +

molinspiration.com/cgi/properties

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### Calculation of Molecular Properties and Bioactivity Score

Calculate Properties

Predict Bioactivity

Galaxy 3D Generator

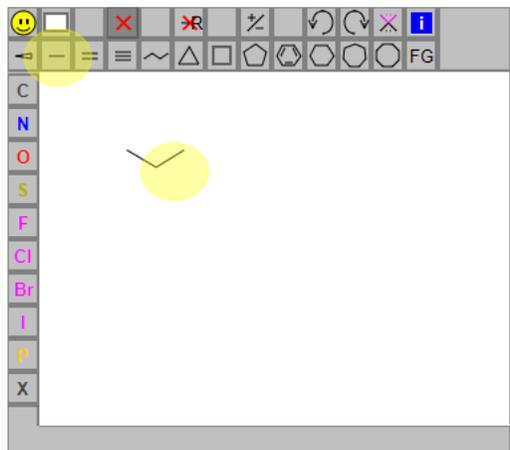
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Diethylene glycol | C<sub>4</sub>H<sub>10</sub>O<sub>3</sub> | C x +

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### Calculation of Molecular Properties and Bioactivity Score

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Predict Bioactivity

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Diethylene glycol | C<sub>4</sub>H<sub>10</sub>O<sub>3</sub> | C x +

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Diethylene glycol | C<sub>4</sub>H<sub>10</sub>O<sub>3</sub> | C x +

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### Calculation of Molecular Properties and Bioactivity Score

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Diethylene glycol | C<sub>4</sub>H<sub>10</sub>O<sub>3</sub> | C x +

pubchem.ncbi.nlm.nih.gov/compound/8117#section=2D-Structure

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Diethylene glycol | C<sub>4</sub>H<sub>10</sub>O<sub>3</sub> | C x +

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### 1.1 2D Structure

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### Calculation of Molecular Properties and Bioactivity Score

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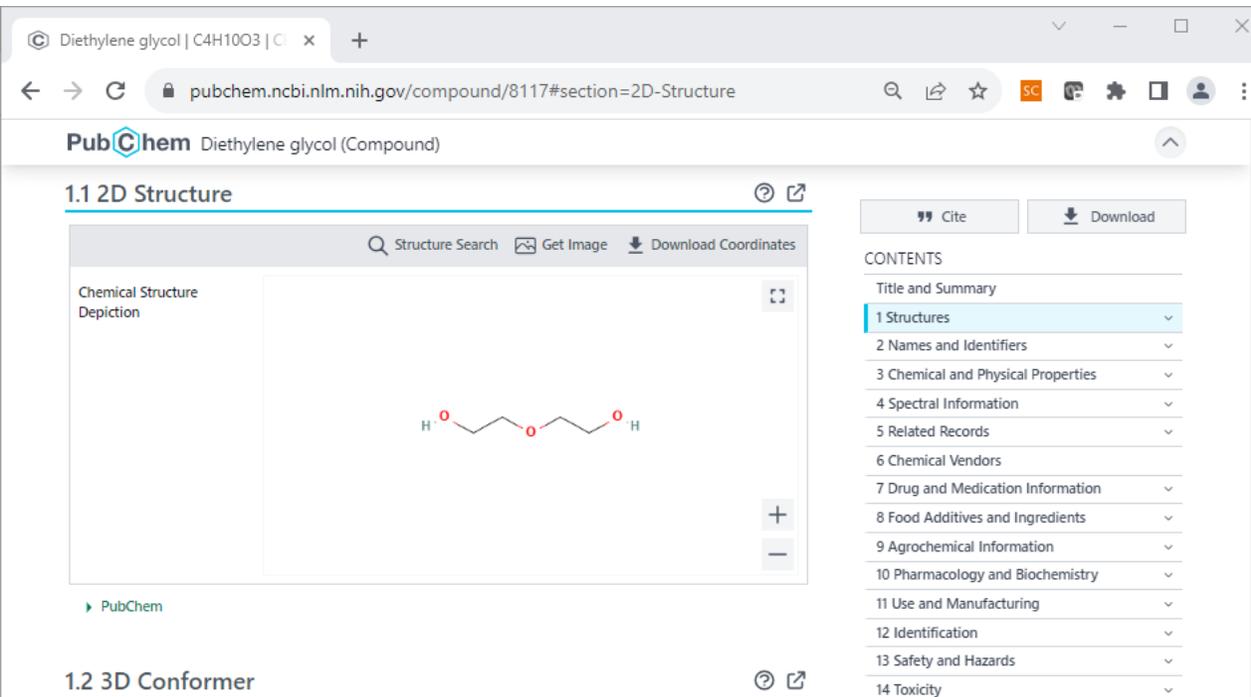
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2D\_structureの書き込みが完了したら  
右欄上端の Calculate Properties をクリックします。



Diethylene glycol | C<sub>4</sub>H<sub>10</sub>O<sub>3</sub> | C x +

pubchem.ncbi.nlm.nih.gov/compound/8117#section=2D-Structure

PubChem Diethylene glycol (Compound)

### 1.1 2D Structure

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Chemical Structure Depiction

OCCOCCO

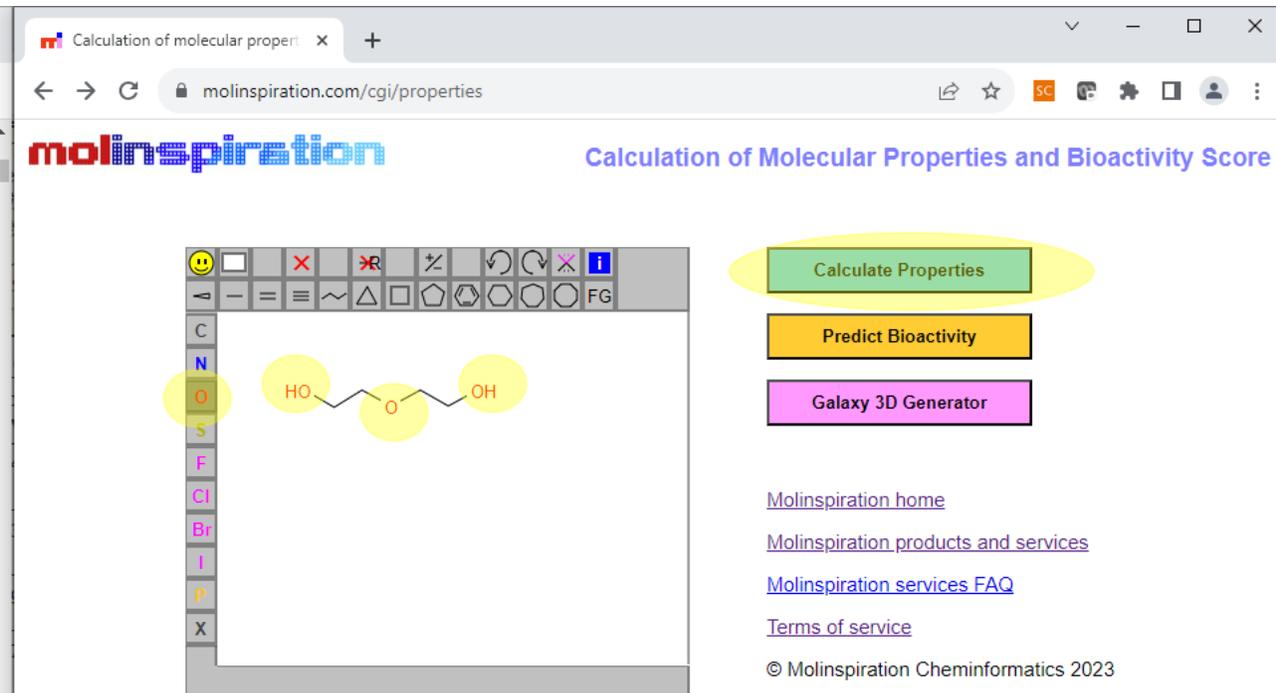
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### 1.2 3D Conformer

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### Calculation of Molecular Properties and Bioactivity Score

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Chemical structure editor showing Diethylene glycol (HO-CH<sub>2</sub>-CH<sub>2</sub>-O-CH<sub>2</sub>-CH<sub>2</sub>-OH) with a toolbar and a vertical element list (C, N, O, S, F, Cl, Br, I, P, X).

Diethylene glycol | C4H10O3 | C x +

pubchem.ncbi.nlm.nih.gov/compound/8117#section=2D-Structure

PubChem Diethylene glycol (Compound)

### 1.1 2D Structure

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Calculation of molecular propert x +

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### Calculation of Molecular Properties

miSMILES: OCCOCCO  
Diethylene glycol

Molinspiration\_property\_engine v2022.08

miLogP	-1.16
TPSA	49.69
natoms	7
MW	106.12
nON	3
nOHNH	2
nviolations	0
nrotb	4
volume	104.86

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[Get 3D geometry](#). BETA

This was request 8 out of 1000 available this month for your site 213.3.44.89  
With technology from Molinspiration you can easily setup similar service also directly on your intranet

ジエチレン・グリコール のproperties(2022\_08) が 表示されます。  
Volume (モル体積) が104.89 mLogP が-1.16 と表記されています。  
これらの情報はSML6のWelle式には不可欠な特性です。

Fig\_03:PubChemデータベースを立ち上げた時の初期画面  
bikoku

移行物質のジエチレン・グリコールを事例とします。  
CAS.No は 111-46-6 です。

モル体積 と Log Powの値を探索します。

最初にPubChem から ジエチレン・グリコール の  
SDFファイルをダウンロードする操作の説明をします。

- ① PubChemを起動するには  
<https://pubchem.ncbi.nlm.nih.gov> を  
立ち上げます。  
左がPubChemの初期画面です。
- ② 赤破線枠にCAS No.の “111-46-6”  
を入力します。

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SEARCH FOR

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**BEST MATCH**

**DIETHYLENE GLYCOL; 111-46-6; 2,2'-Oxydiethanol; Diglycol; 2,2'-Oxybisethanol; 2-(2-Hydroxyethoxy)ethanol; Diethylenglykol; Digol; ...**

Compound CID: 8117

MF: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub> MW: 106.12g/mol

IUPAC Name: 2-(2-hydroxyethoxy)ethanol

Isomeric SMILES: C(COCCO)O

InChIKey: MTHSVFCYNBDYFN-UHFFFAOYSA-N

InChI: InChI=1S/C4H10O3/c5-1-3-7-4-2-6/h5-6H,1-4H2

Create Date: 2005-03-26

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(1)

[Substances](#)  
(119)

[Literature](#)  
(5)

Searching chemical names and synonyms including IUPAC names and InChIKeys across the compound collection. Note that annotations text from compound summary pages is not searched. [Read More...](#)

**1 result**

**DIETHYLENE GLYCOL; 111-46-6; 2,2'-Oxydiethanol; Diglycol; 2,2'-Oxybisethanol; ...**

Compound CID: 8117

MF: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub> MW: 106.12g/mol

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Create Date: 2005-03-26

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ACTIONS ON RESULTS WITH ID TYPE:

Compounds

Push to Entrez
🔗

Save for Later
▼

Linked Data Sets
▼

**Compounds**  
(1)**Substances**  
(119)**Literature**  
(5)

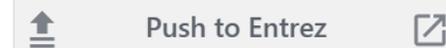
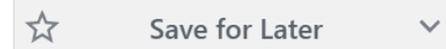
Searching chemical names and synonyms including IUPAC names and InChIKeys across the compound collection. Note that annotations text from compound summary pages is not searched. [Read More...](#)

1 result

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ACTIONS ON RESULTS WITH ID TYPE:

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Push to EntrezSave for LaterLinked Data Sets**DIETHYLENE GLYCOL; 111-46-6; 2,2'-Oxydiethanol; Diglycol; 2,2'-Oxybisethanol; ...**

Compound CID: 8117

MF:  $C_4H_{10}O_3$  MW: 106.12g/mol

IUPAC Name: 2-(2-hydroxyethoxy)ethanol

Isomeric SMILES: C(COCCO)O

InChIKey: MTHSVFCYNBDYFN-UHFFFAOYSA-N

InChI: InChI=1S/C4H10O3/c5-1-3-7-4-2-6/h5-6H,1-4H2

Create Date: 2005-03-26

[Summary](#)[Similar Structures Search](#)[Related Records](#)

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Summary (Search Results)

CSV JSON XML

COMPRESSION:

None  GZip

Chemical Structure Records

SDF JSON XML ASNT

COORDINATE TYPE:

2D  3D

COMPRESSION:

None  GZip

Chemical Structure Images

- ④ 目標とするDownloadはSDF(Structure Design File)です。赤線枠のSDF をクリックします。
- ⑤ Download が開始されます。PubChemデータベースからSDFファイル入手することができました。なおファイルの属性はTXTですので、TXTファイルとして取り込みます。

ダウンロード

PubChem\_compound\_text\_111-46-6\_records.sdf

[ファイルを開く](#)

[もっと見る](#)

```
PubChem_compound_text_111-46-6_records - メモ帳
ファイル(E) 編集(E) 書式(O) 表示(V) ヘルプ(H)
8117
-OEChem-11152320422D
17 16 0 0 0 0 0 0 0999 V2000
5.1350 -0.2500 0.0000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.7331 0.2500 0.0000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2.5369 0.2500 0.0000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
6.0010 0.2500 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
4.2690 0.2500 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
6.8671 -0.2500 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.4030 -0.2500 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
6.3996 0.7249 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5.6025 0.7249 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
4.6675 0.7249 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.8705 0.7249 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
6.4685 -0.7249 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.2656 -0.7249 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.0044 -0.7249 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.8015 -0.7249 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.2700 -0.0600 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2.0000 -0.0600 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1 4 1 0 0 0 0 0
1 5 1 0 0 0 0 0
2 6 1 0 0 0 0 0
2 16 1 0 0 0 0 0
3 7 1 0 0 0 0 0
3 17 1 0 0 0 0 0
4 6 1 0 0 0 0 0
4 8 1 0 0 0 0 0
4 9 1 0 0 0 0 0
5 7 1 0 0 0 0 0
5 10 1 0 0 0 0 0
5 11 1 0 0 0 0 0
6 12 1 0 0 0 0 0
6 13 1 0 0 0 0 0
7 14 1 0 0 0 0 0
7 15 1 0 0 0 0 0
M END
> <PUBCHEM_COMPOUND_CID>
0117
<
```

- ⑥ DownloadされたファイルはTXTファイルです。  
ワードパッドあるいはメモ帳で表示させます。  
左図はメモ帳の表示例です。  
ここで表示させる意味はないのですが、111-46-6の  
化学構造がテキストファイルの内容を確認しています。

SDFファイル名はCAS.Noが含まれており識別が容易です。

PubChem\_compound\_text\_111-46-6\_records.sdf

- ⑦ 次にmolinspirationを起動します。  
**molinspiration**のURLは  
<https://molinspiration.com/cgi-bin/properties>

- 下図はmolinspirationの起動後の画面です。  
⑧ここで赤破線枠内にカーソルを置いて**Right\_Click** します。

Calculate Properties

Predict Bioactivity

Galaxy 3D Generator

[Molinspiration home](#)

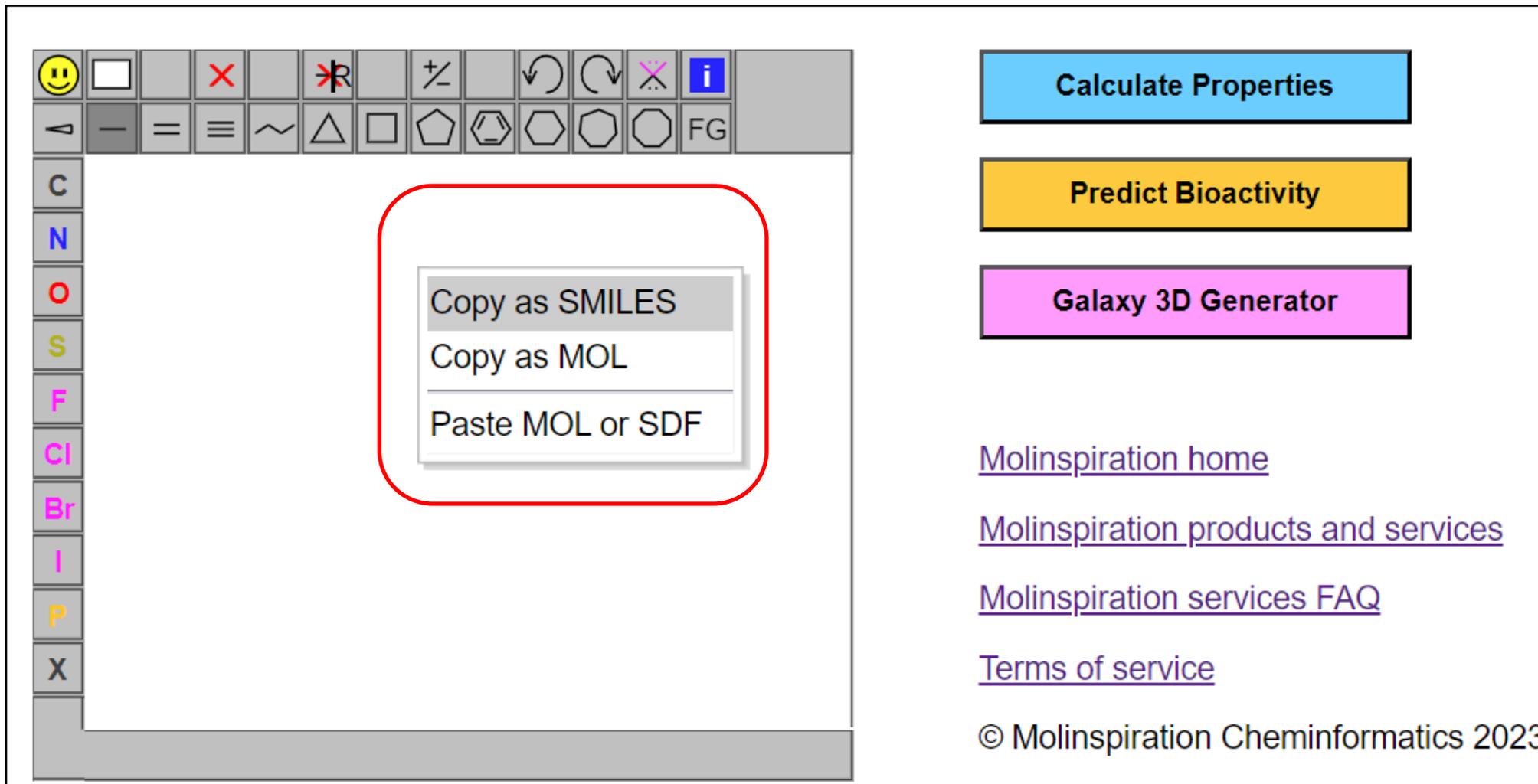
[Molinspiration products and services](#)

[Molinspiration services FAQ](#)

[Terms of service](#)

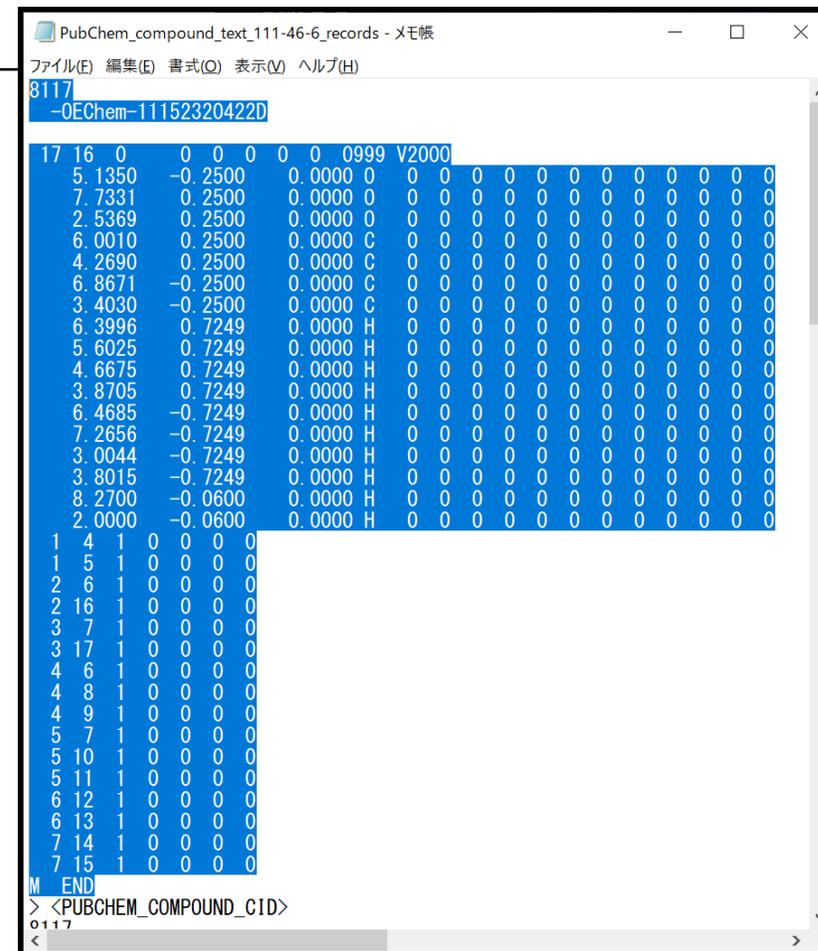
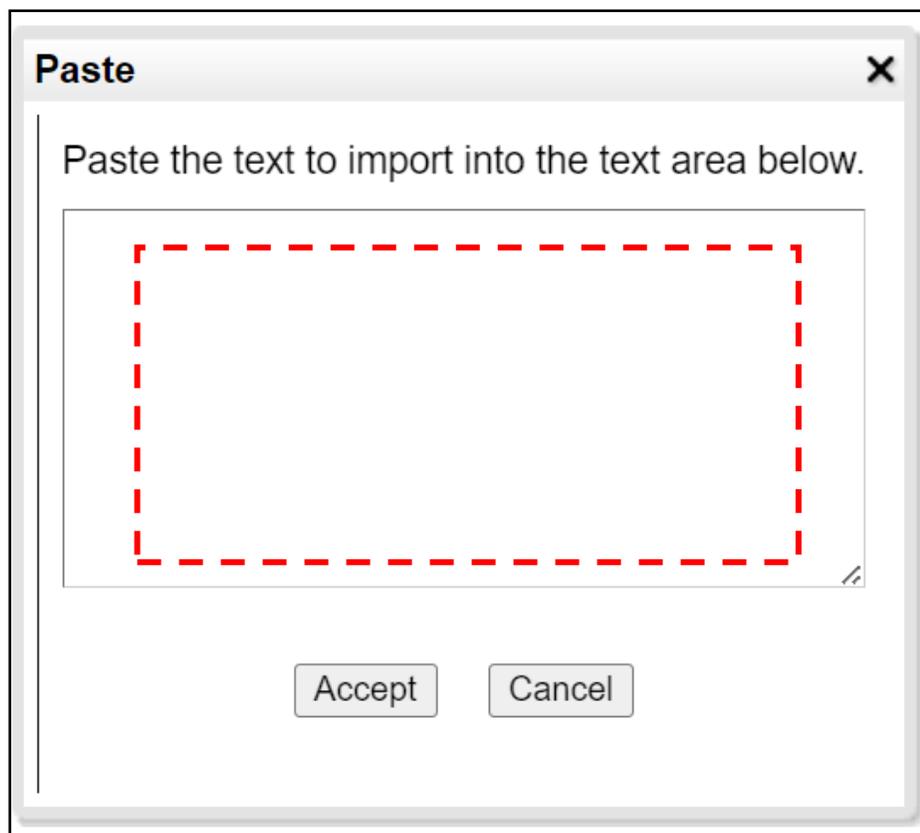
© Molinspiration Cheminformatics 2023

- ⑧ここで赤破線枠内にカーソルを置いて**Right\_Click** すると 赤線枠が表示されます。
- ⑨ Paste MOL or SDF を選択します。

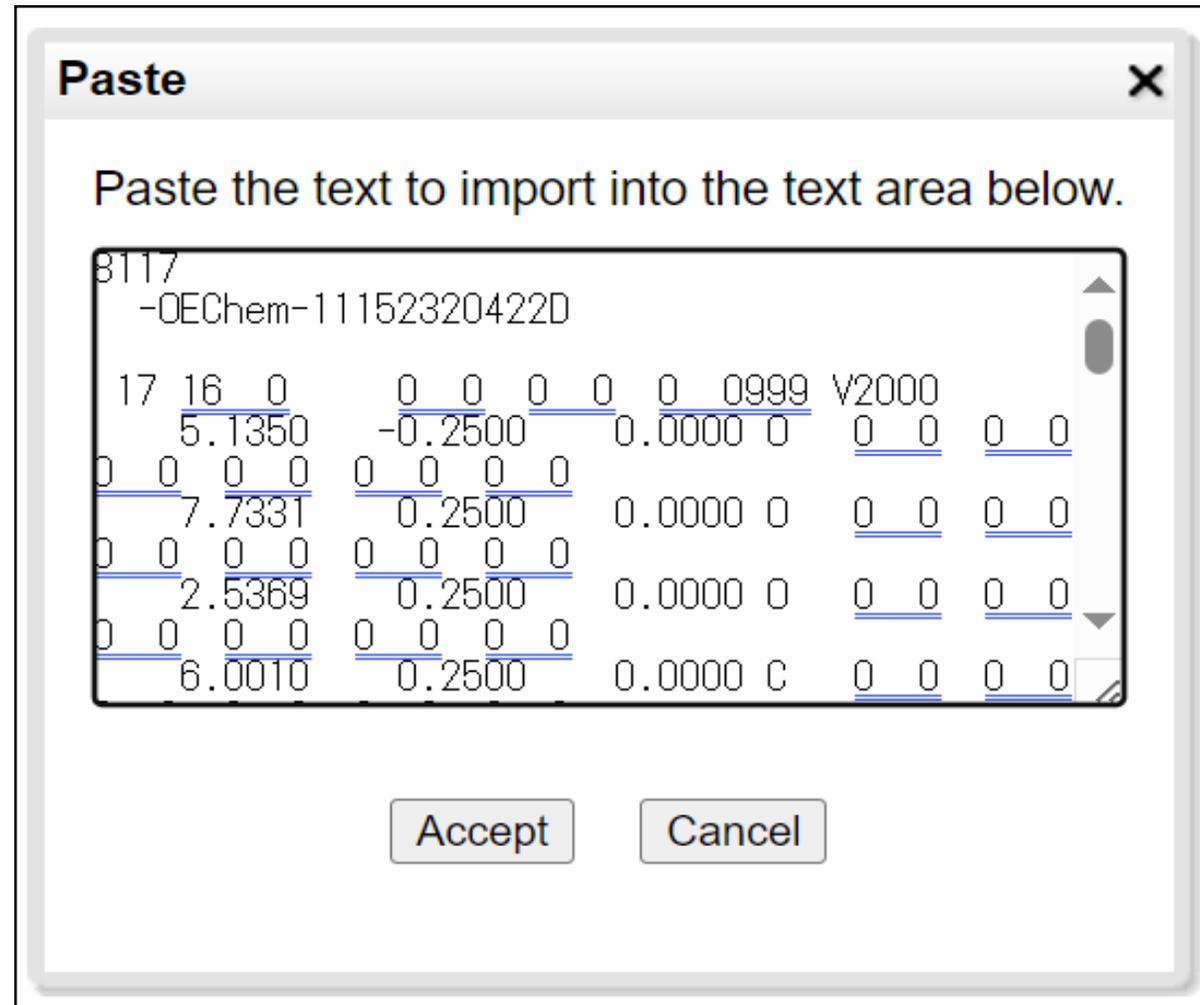


The screenshot displays the Molinspiration software interface. On the left, there is a toolbar with various icons for editing and drawing. Below the toolbar is a vertical menu with chemical symbols: C, N, O, S, F, Cl, Br, I, P, X. The main workspace contains a context menu with three options: "Copy as SMILES", "Copy as MOL", and "Paste MOL or SDF". The "Paste MOL or SDF" option is highlighted with a red rounded rectangle. To the right of the workspace, there are three large buttons: "Calculate Properties" (blue), "Predict Bioactivity" (yellow), and "Galaxy 3D Generator" (pink). Below these buttons are several hyperlinks: "Molinspiration home", "Molinspiration products and services", "Molinspiration services FAQ", and "Terms of service". At the bottom right, there is a copyright notice: "© Molinspiration Cheminformatics 2023".

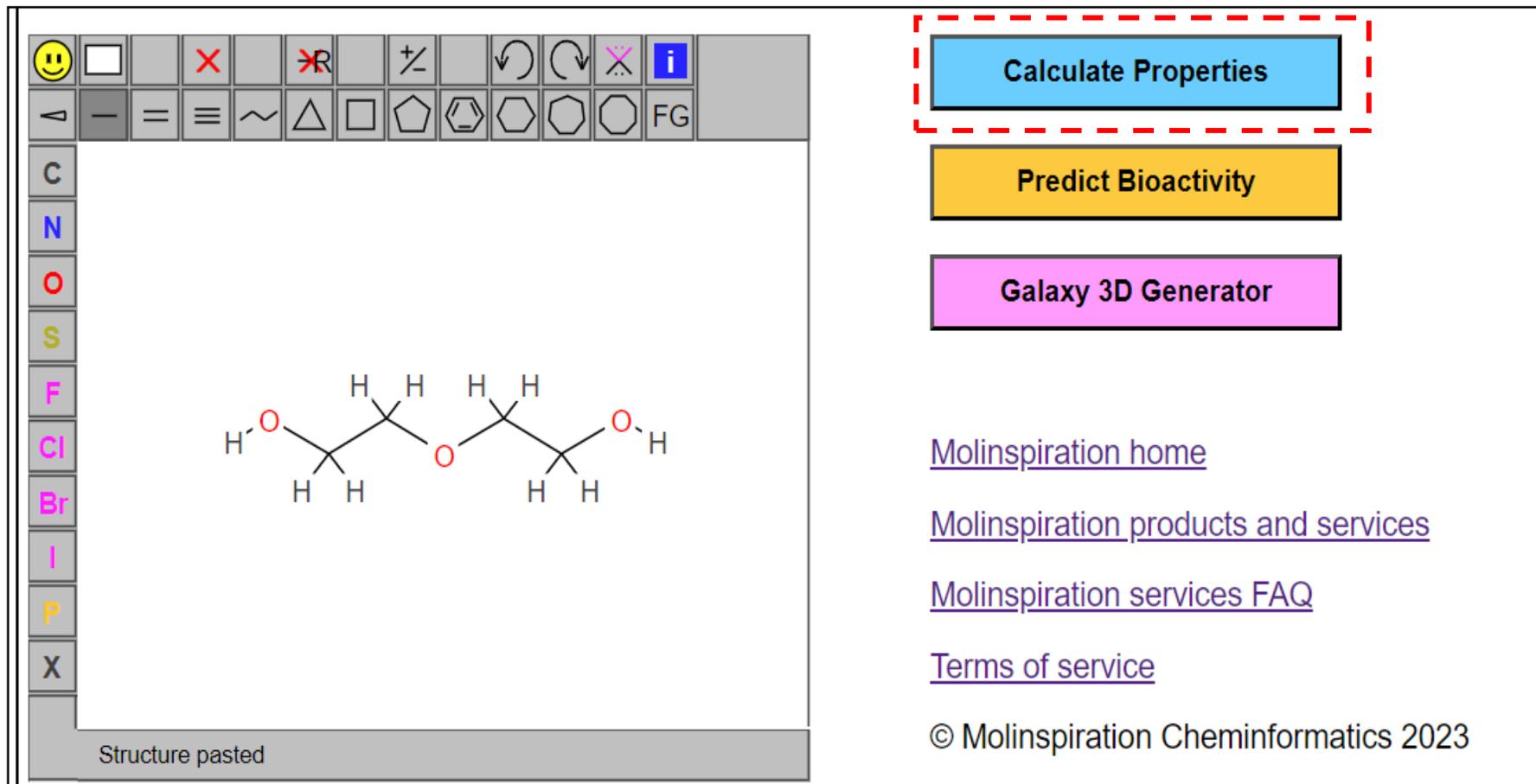
- ⑩ Paste MOL or SDF を Clickします。左図が表示されるので赤破線枠内にSDFファイルをPasteします。ただしPasteするときはFig\_05のテキスト表示した状態でテキストファイルをペーストすることが必要です。SDFファイルをコピーしてからペーストするのではなく、テキストをベタコピーしてからペーストすることが必要です。Copy & Pasteしたら、左・下図のAccept をclickします。



- ⑪ Copy & Pasteしたら、Accept をclickします。



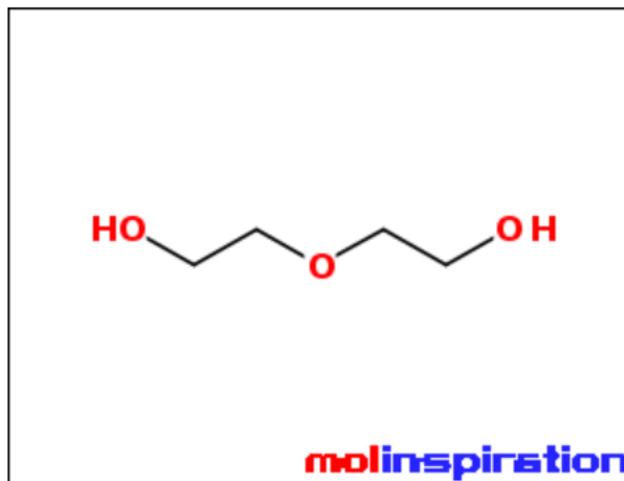
SDFファイルをテキストファイルで表示してから Copy & Paste して、Acceptをクリックすると操作完了です。  
ジエチレン・グリコールの化学構造を ChemDrawのように操作をしなくても、2Dno化学構造図が入力完了！  
化学特性を探索するための入力作業が完了しました。  
最後に ⑫赤破線枠のCalculate Properties をクリックします。



The screenshot displays a chemical structure editor interface. On the left, a vertical toolbar contains buttons for elements: C, N, O, S, F, Cl, Br, I, P, and X. The main workspace shows the chemical structure of ethylene glycol (1,2-ethanediol) with all atoms and bonds explicitly drawn. Below the structure, the text "Structure pasted" is visible. On the right side, a sidebar contains three buttons: "Calculate Properties" (highlighted with a red dashed border), "Predict Bioactivity", and "Galaxy 3D Generator". Below these buttons are several hyperlinks: "Molinspiration home", "Molinspiration products and services", "Molinspiration services FAQ", and "Terms of service". At the bottom right of the sidebar, the copyright notice "© Molinspiration Cheminformatics 2023" is present.

## molinspiration

miSMILES: [H]OC([H])([H])C([H])([H])OC([H])([H])C([H])([H])O[H]  
Diethylene glycol



[Molinspiration property engine](#) v2022.08

<a href="#">miLogP</a>	-1.16
<a href="#">TPSA</a>	49.69
<a href="#">natoms</a>	7
<a href="#">MW</a>	106.12
<a href="#">nON</a>	3
<a href="#">nOHNH</a>	2
<a href="#">nviolations</a>	0
<a href="#">nrotb</a>	4
<a href="#">volume</a>	104.86

[Get data as text](#) (for copy / paste).

[Get 3D geometry](#) BETA

This was request 2 out of 1000 available this month for your site 123.217.197.242  
With technology from Molinspiration you can easily setup similar service also directly on your intranet.  
Comments or questions ? See our [FAQ](#) and do not hesitate to provide feedback or contact us by email !

[New molecule](#) [Predict bioactivity](#) [About properties](#) [Molinspiration home](#)

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SML6のWelle式アプローチでは  
下記2項目が最も必要とする物性値です。

Log\_Pow : -1.16  
モル体積 : 104.86





Palmetrics