Balancing Chemical Equations and Calculation of Molecular Weight

MatDeck can be used to obtain the molecular formula of a compound by its name, IUPAC name, or SMILES. In this example we show Ethanol fermentation, also called alcoholic fermentation, which converts sugars such as glucose into ethanol and carbon dioxide. Therefore, we need the molecular formula of Glucose, Ethanol, and Carbon dioxide, which is obtained by using our Graphical Chemical Tool. The formula is obtained as a string, and can be stored as a variable. The Chemical Tool form is inserted from the Insert menu, using Select Form, which is at the far right side of the Insert menu. Before the Chemical Tool is obtained within a document, users can specify the names of the variables in the appropriate tool.

$$\text{form15652} := \text{CHEMICAL\_INFO\_Form}(\text{"form15652"})$$

Chemical Tool

SMILES String

OC[C@@H](O)[C@@H](O)[C@H](O)[C@@H](O)C=O

Get by SMILES

IUPAC name or Common Name

(2R,3S,4R,5R)-2,3,4,5,6-pentahydroxyhexanal

Get by Name

Molecular Formula

C6H12O6

Common Names

Molecular mass

99.99
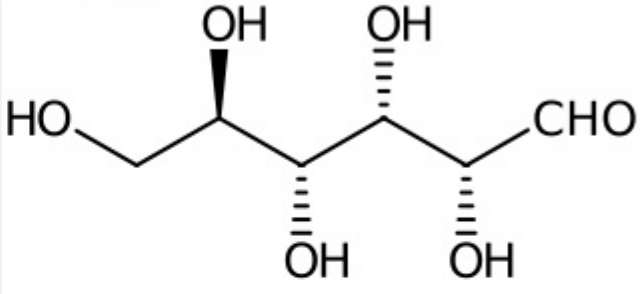
Molecular Image

$$\text{smiles15652} := \text{chemical\_info\_smiles}(\text{form15652})$$

$$\text{iupac15652} := \text{chemical\_info\_iupac}(\text{form15652})$$

$$\text{Glucosef} := \text{chemical\_info\_formula}(\text{form15652})$$

$$\text{Glucosem} := \text{chemical\_info\_mmass}(\text{form15652})$$

Next, we will obtain the chemical formula and other important data about Ethanol. The Chemical Tool allows us to change variable names which we will use this time. We also need data about CO_2. Variables which are not needed can be changed or removed. We can move expressions within a canvas to format the document.

form30179 := CHEMICAL_INFO_Form("form30179")

Chemical Tool

SMILES String

CCO

[Get by SMILES]

IUPAC name or Common Name

ethanol

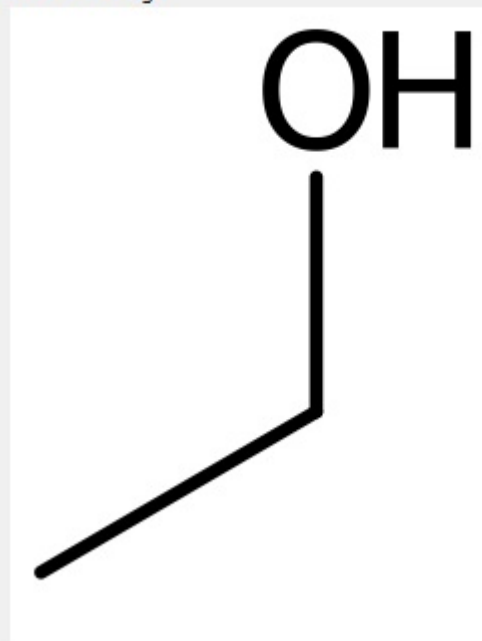[Get by Name]

Molecular Formula

C2H6O

Common Names

[▼]

Molecular mass

46.07 ⬍

Molecular Image

Ethanolf := chemical_info_formula(form30179)
Ethanolm := chemical_info_mmass(form30179)

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form2682 := CHEMICAL_INFO_Form("form2682")

Chemical Tool

SMILES String

O=C=O

[Get by SMILES]

IUPAC name or Common Name

carbon dioxide

[Get by Name]
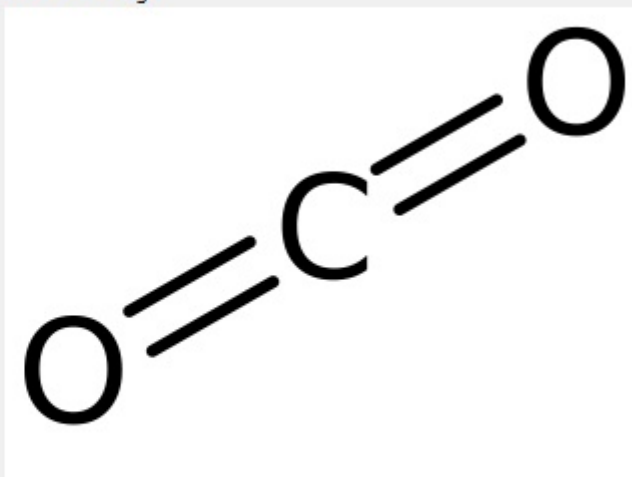
Molecular Formula

CO2

Common Names

[▼]

Molecular mass

44.01 ⬍

Molecular Image

CO2f := chemical_info_formula(form2682)
CO2m := chemical_info_mmass(form2682)

MatDeck comes implemented with several functions that can help you determine if a chemical equation is feasible or not, and help you balance the equation if a reaction is feasible. There is an easy way to balance equations. The procedure is given in two steps:

- Create the equation that you want to be balanced, Use the Ctrl. + = key combination to create an equal sign.
- Position the mouse cursor above the equal sign and right click the Equal sign, it will transform to a dart and the equation will be balanced (if reaction is feasible).

However, chemical equations are expected to be symbolic. Therefore, we have to convert string formulas into symbolic values, which is done using the str2symbol(variable, true/false) function. Here the variable is a string value which is converted to a symbolic value, and the other argument is used as true if we want to skip spaces in a given string. The formula in the canvas is obtained by converting string variables into symbolic values.

$$C6H12O6 \rightarrow 2\ C2H6O + 2\ CO2$$

Molecular Weight used in calculation

We have easily obtained the molecular mass of all compounds used in a chemical reaction directly from the Chemical Tool. Next, we can calculate how much Ethanol we can get from **1g** of Glucose. We can use the balanced equation obtained above, and their molecular weights to perform calculus.

$$mEthanol := \frac{2 \cdot Ethanolm}{Glucosem} \cdot 1\ gr$$

$$mEthanol = 0.921\ gr$$