

Introduction and General Background

IUCLID 5.5 BASICS

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Content

- What is IUCLID and where to find it
- Definition of important terms

What is IUCLID 5?

- IUCLID 5 is an IT application built to store, organize and report on the hazardous properties of chemicals. IUCLID 5 is intended to serve this purpose for both REACH and other chemical legislative programmes (e.g. OECD HPV and EU Biocides)
- Industry uses IUCLID 5 to prepare data for submission to ECHA to fulfill their obligations under REACH
- IUCLID 5 is used by the Agency both for Agency staff and Member States Competent Authorities (MSCAs)

Where to get IUCLID 5

IUCLID 5 is available free of charge on the IUCLID 5 website at <http://echa.europa.eu/IUCLID>



also accessible via the ECHA website



Download



Download IUCLID version 5.5

[Stand-alone version 5.5.0](#)

[Distributed version 5.5.0](#)

[CSR Plug-in](#)

[Dissemination Plug-in](#)

[Fee Calculation Plug-in](#)

[Help System Plug-ins](#)

[Query Plug-in](#)

[Technical Completeness
Check \(TCC\) Plug-in](#)

Stand-alone version 5.5.0

Installer for Windows (version 5.5.0)

This package contains a java program which helps the user installing IUCLID 5 through a simple graphical interface. Before you start the installation of IUCLID 5 you need to install separately Java 6 or 7 and PostgreSQL 9.0.

[Download the installation package >](#)

Manual installation (version 5.5.0)

This package contains all files needed to set up manually a stand-alone IUCLID application. Recommended for expert users and when specific configuration is required.



[Download the installation package >](#)

EC inventory

- **What is it?**
- The **EC inventory** (the chemicals identifiers catalogue) is a list of substance identities which is based on a combination of the following EU inventories: EINECS, ELINCS and NLP-list.

Information contained

EC inventory

EC number	<input type="text" value="233-162-8"/>	CAS number	<input type="text" value="10049-04-4"/>	 
EC name	<input type="text" value="chlorine dioxide"/>			
Molecular formula	<input type="text" value="ClO2"/>			
Description	<input type="text"/>			

- EC number
- EC name
- CAS number
- Molecular formula
- Description



The screenshot shows the IUCLID 5 website interface. At the top left is the IUCLID 5 logo with the text 'INTERNATIONAL UNIFORM CHEMICAL INFORMATION DATABASE'. At the top right, a user is logged in as 'Martin Albert (mralbi)' with a 'Logout' link. Below this is a horizontal navigation menu with the following items: Home, IUCLID 5 Project, User Info, Download, Support (circled in red), REACH, and News. Below the navigation menu is a secondary menu with the following items: Documentation, Training, Links, Get Reference substances, IUCLID format, FAQ, ECHA Helpdesk Contact, and Get EC Inventory (circled in red).

Get EC Inventory

In your work with IUCLID 5, you will see that the system will often prompt you for 'EC inventory' information. The EC Inventory is a list of substance identities which is based on a combination of the following EU inventories: EINECS, ELINCS and NLP-list. It is recommended to download and import the complete EC inventory into your IUCLID 5 installation. Please go to the link below to do so.

Download [EC Inventory version 1.2 \(English\)](#)

Import

To import the new EC inventory and/or the 'list numbers' into your IUCLID installation:

- *Open IUCLID*



Reference substance

In IUCLID 5, the chemical composition of a Substance is defined by linking it to Reference substance(s) that each define one of the following:

- **Overall Substance identity and**
 - **Constituent(s)**
 - **Impurity(ies)**
 - **Additive(s)**



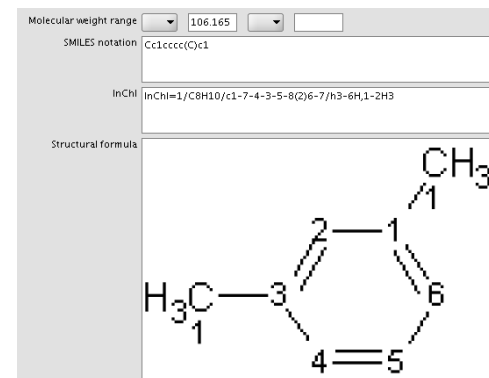
Information in a Reference Substance

- Name(s), EINECS, ELINCS, CAS, Composition...
[Identity of the substance Art 10 (a) (ii) – Annex VI, section 2]
- Direct link to EC inventory (if possible)

EC inventory

EC number	233-162-8	CAS number	10049-04-4		
EC name	chlorine dioxide				
Molecular formula	ClO2				
Description					

- Reference substance gives information on the substance identity e.g. IUPAC name and molecular and structural information, including SMILES notation, InCHI, etc.



**IUCLID 5**
INTERNATIONAL UNIFORM CHEMICAL INFORMATION DATABASE[Home](#) | [IUCLID 5 Project](#) | [User Info](#) | [Download](#) | [Support](#) | [REACH](#) | [News](#)[Documentation](#) | [Training](#) | [Links](#) | [Get Reference substances](#) | [IUCLID format](#) | [FAQ](#) | [ECHA Helpdesk Contact](#) | [Get EC Inventory](#)

Get Reference substances

In your work with IUCLID 5, you will see that you will often be prompted for "Reference substance" information. A Reference substance is a "label" to be attached to each of your substances in IUCLID 5. Each "Reference substance", in turn, features several data elements that unequivocally identify a substance. In order to make your work easier, the IUCLID 5 Support Team has prepared Reference substance data for tens of thousands of substances, and you can download one, several, or all of them and then import them into your IUCLID 5. Please use the links below to select the Reference substance(s) you need, and to download them. Keep the downloaded files in a safe place like you did with the LEOX file, until you need to import them into your local IUCLID 5.

[Download](#) the full set of References substances [407Mb]
This file includes 68,679 substances listed on EINECS

[Download](#) the reduced list of Reference substances (Recommended version) [22,7Mb]
This file includes the 3,776 most commonly used substances

[Select and download](#) a Subset of References substances
With this option, you will be able to build your own selection of Reference substances

First steps wizard

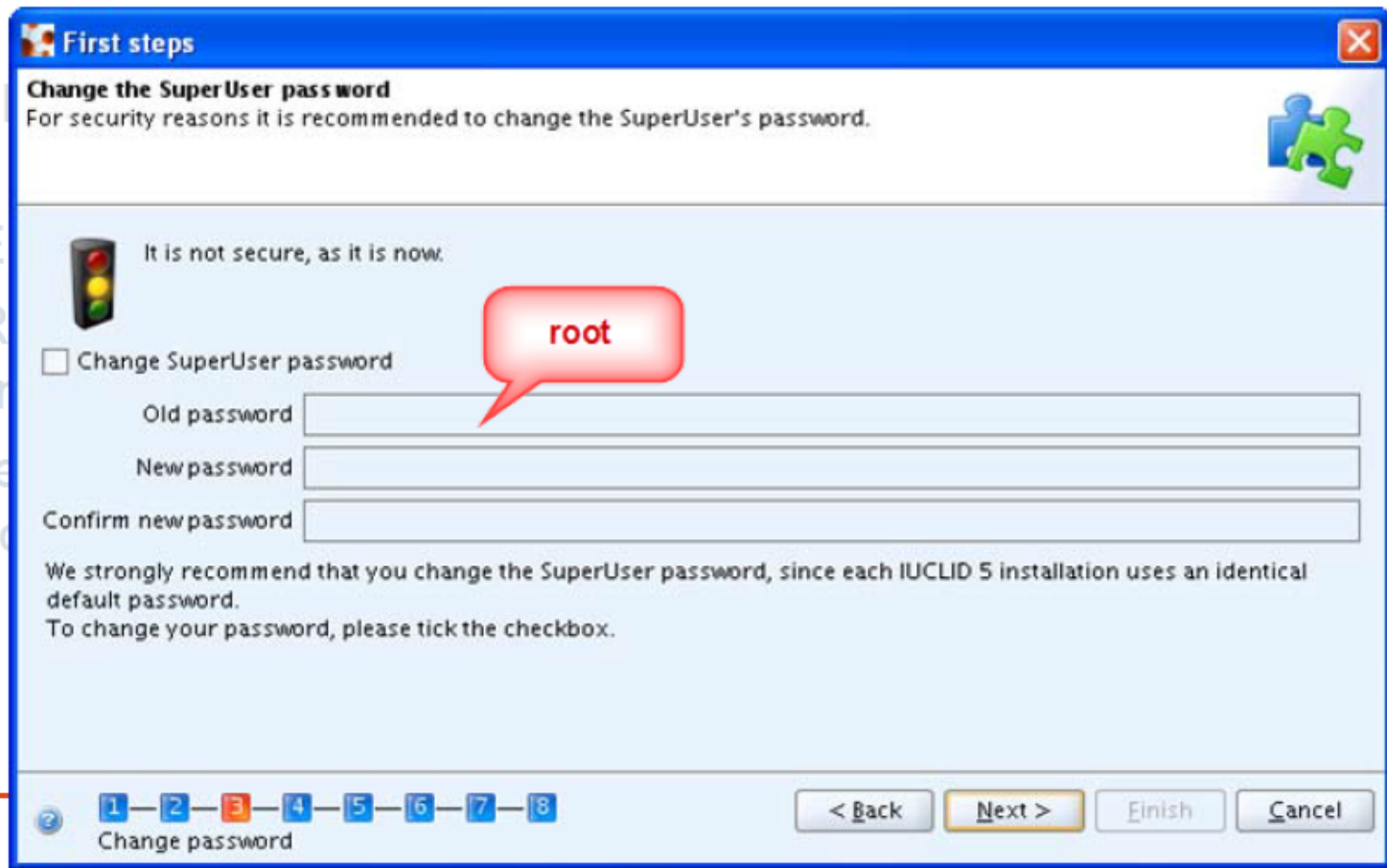
1. Change the SuperUser password

2. Import your information

3. Import the E


4. Import the R
Substance in

5. Create a user
and define r



First steps

Change the SuperUser password
For security reasons it is recommended to change the SuperUser's password.

 It is not secure, as it is now.

Change SuperUser password

Old password

New password

Confirm new password

We strongly recommend that you change the SuperUser password, since each IUCLID 5 installation uses an identical default password.
To change your password, please tick the checkbox.

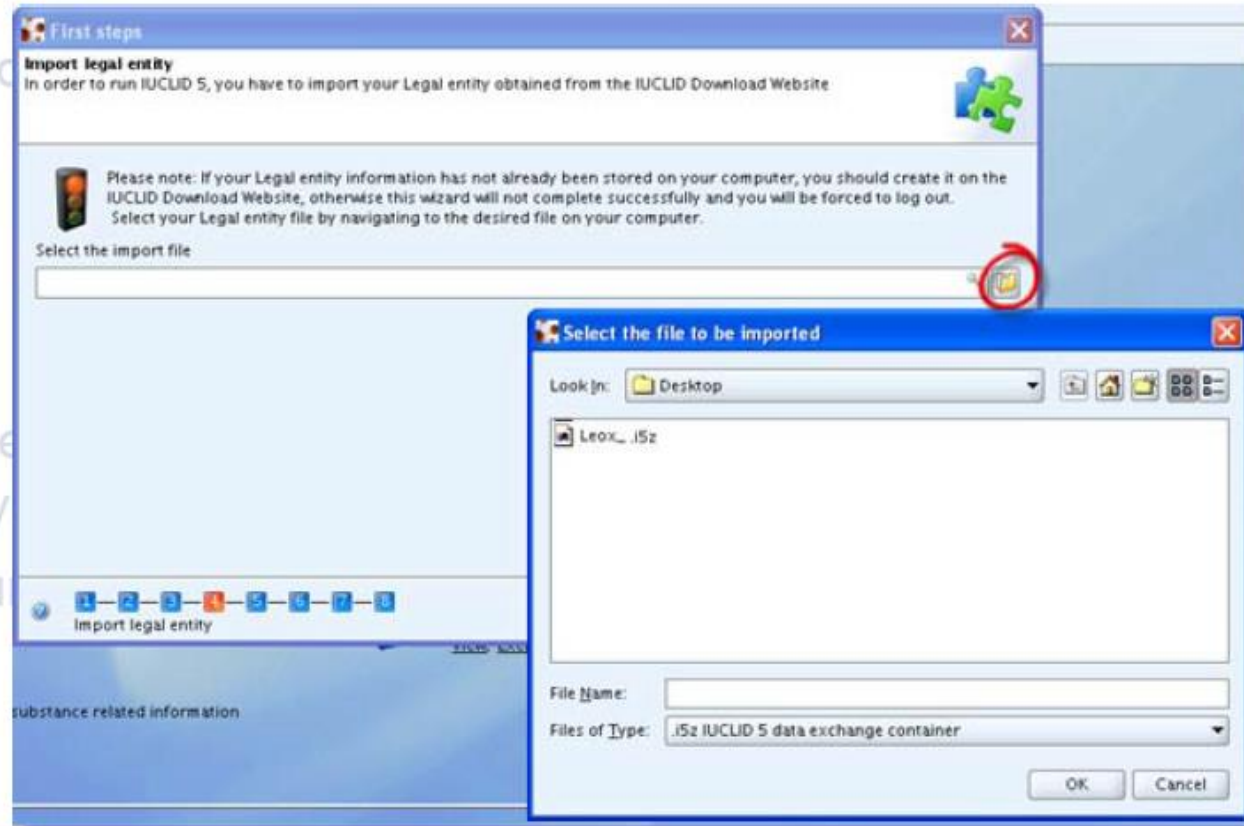
1 — 2 — 3 — 4 — 5 — 6 — 7 — 8
Change password

< Back Next > Finish Cancel



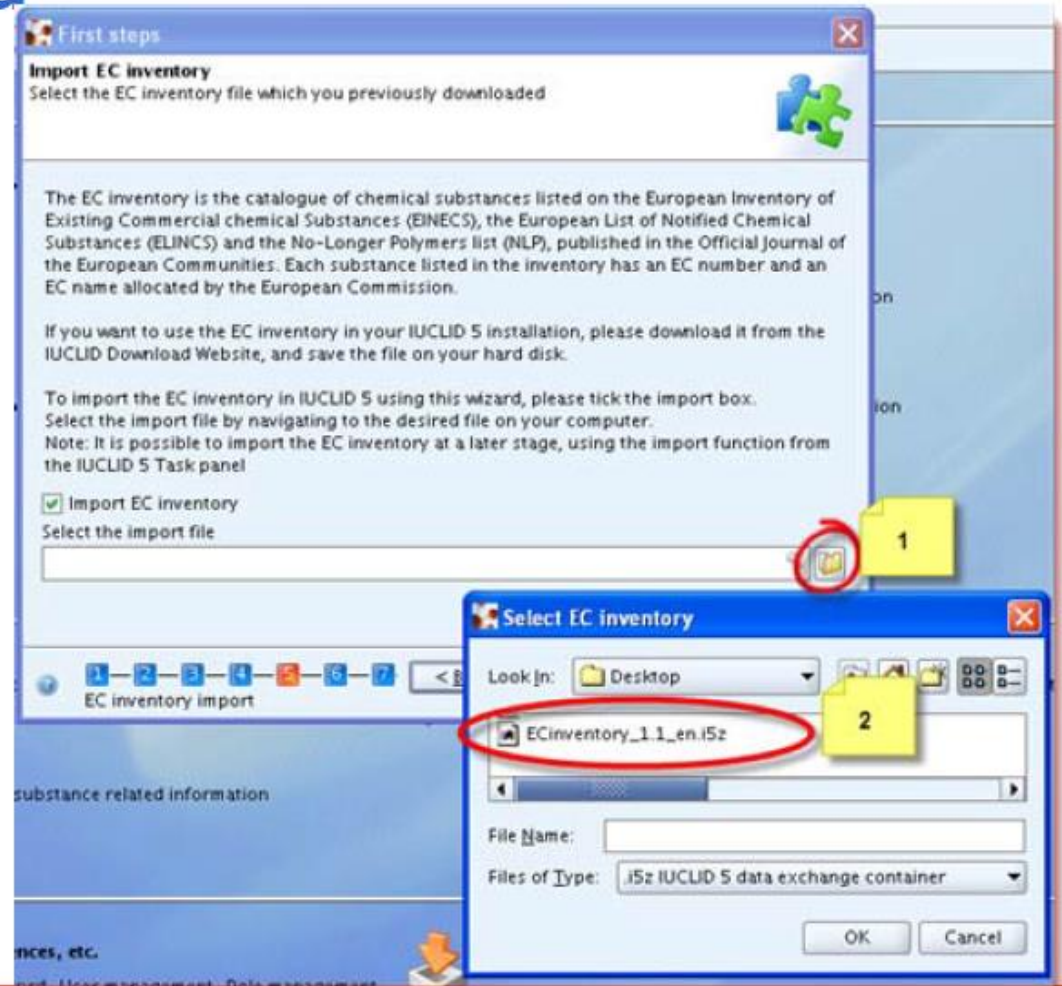
First steps wizard

1. Change the SuperUser password
- 2. Import your Legal Entity information**
3. Import the EC inventory
4. Import the Reference Substance inventory
5. Create a user account and define roles



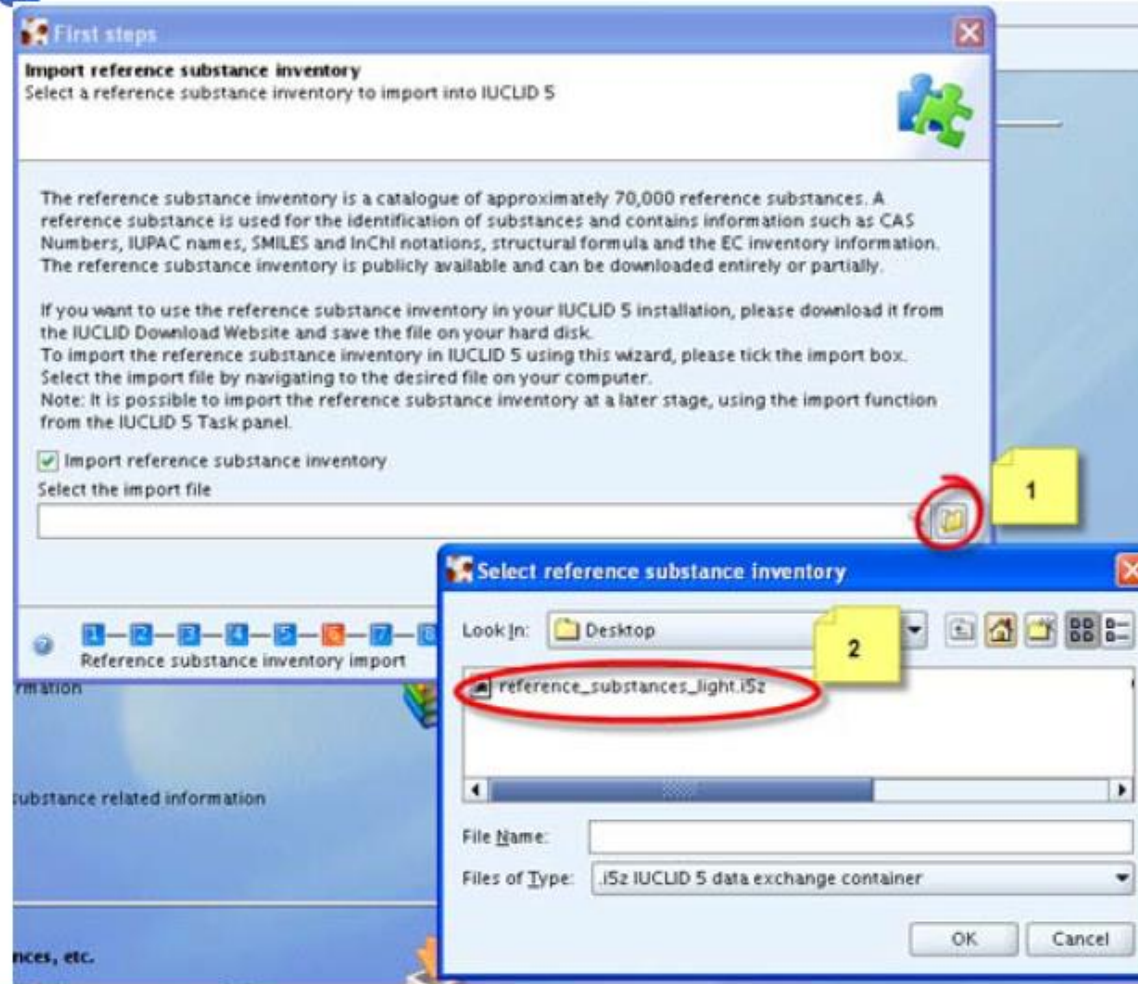
First steps wizard

1. Change the SuperUser password
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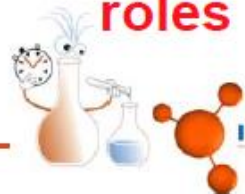
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First steps wizard

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- 5. Create a user account and define roles**



IUCLID 5

First steps
Create user account and assign role
It is recommended to create a user account before running IUCLID 5

The SuperUser account is for user administration only, and therefore to run IUCLID 5 we strongly recommend that you create your own user account by selecting the following tick box. Assign your role and legal entity and specify the attachments and import/export directories.

Create user

Login name: (newuser)

Full name: _____

Set password

Unassigned roles:
Administrator
Full access
Read-only

Assigned roles: _____

Assigned legal entities: _____

Query
Search for legal entities that will be assigned to the user.
Note: Only official entities (OLEO) that have been created in IUCLID Download web interface can be assigned to a user.

Legal entity name: _____
Town: _____
Country: _____

Show only active values Search

Name	E-mail	Address
ECHA Helpdesk / Helsinki / Finland		Helsinki, Finland

Attachments directory: _____
Import/export directory: _____

Assign Cancel

1 2 3 4 5 6 7 8
Create user

< Back Next > Finish Cancel



Definition of a Substance

A **Substance** is a regulatory concept designed to contain as much as possible of the information about a chemical product that is relevant to chemical regulation.

For example:

- the precise chemical composition
- toxicological data
- guidance on its safe use

A “**Substance data set**” is the central core of information in IUCLID that is used to store the data of a Substance.



Defining Chemical Composition

Constituent

A substance typically contains either one or a small number of different principal ingredients that each have a single or narrowly defined molecular structure.

Impurity

The nature of chemical manufacture means that there are unwanted ingredients.

Additive

Sometimes, an ingredient is added deliberately in small quantities to perform a specific function, such as a stabiliser.



Chemical Composition of a Substance

- A particular molecule might be present in many Substances. For the sake of efficiency, the chemical identity is defined only once. This is done in a Reference substance.
- A Reference substance typically has a single or narrowly defined molecular structure.
- For example, an impurity in one substance might be a constituent of another.

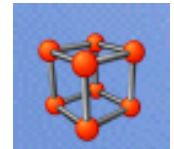


Reference Substance in 1.1

Identification – only one entry

The screenshot displays the ECHA REACH database interface. On the left, a navigation pane shows a tree structure of sections. The '1.1 Identification' section is highlighted with a red oval, and a red arrow points from it to the main content area. The main content area is titled 'Substance: 1,2-Benzenedicarboxylic acid, di-C7-11-branched an' and contains the following sections:

- Substance identification**
 - Chemical name: 1,2-Benzenedicarboxylic acid, di-C7-11-branched an
 - Public name: [Empty field]
 - Legal entity flags: [Flag icon]
 - Legal entity: Example Company 1 / Example city / Finland
 - Third party flags: [Flag icon]
 - Third party: [Empty field]
- Role in the supply chain**
 - Role flags: [Flag icon]
 - Role: Manufacturer Importer Only rep
- Reference substance**
 - Structure icon: [Icon]
 - Structure name: triphenylene / triphenylene / 217-59-4
 - EC number: 205-922-9
 - EC name: triphenylene
 - CAS number: [Empty field]
 - CAS name: [Empty field]



Reference Substance in 1.2

Composition

The screenshot displays the ECHA database interface. On the left, a 'Navigation' pane shows a tree structure with '1.2 Composition' circled in red. Two red arrows point from this circle to the 'Constituents' and 'Impurities' sections of the main data panel on the right.

Navigation Pane:

- 0 Related Information
- 1 General Information
 - 1.1 Identification
 - 1.2 Composition**
 - 1.3 Identifiers
 - 1.4 Analytical information
 - 1.5 Joint submission
 - 1.6 Sponsors
 - 1.7 Suppliers
 - 1.8 Recipients
 - 1.9 Product and process oriented information
- 2 Classification and Labelling
- 3 Manufacture, use and exposure
- 4 Physical and chemical properties

Constituents Panel:

<= 100 % (w/w) 1,2-Benzenedicarboxylic acid, di-C7-11-branched and linear

Reference substance: 1,2-Benzenedicarboxylic acid, di-C7-11-branched and linear

EC number	EC name
271-084-6	1,2-Benzenedicarboxylic acid
CAS number	CAS name
68515-42-4	1,2-Benzenedicarboxylic acid
IUPAC name	

Typical concentration: [dropdown] [input] [dropdown]

Concentration range: [dropdown] [input] <= [input] 100

Remarks: [input]

Impurities: [input]

Additives: [input]

Thank you

