

**ISSBIOC database on carcinogenicity and mutagenicity of biocides and plant protection products (or pesticides).**

**Definition of the fields in files *ISSBIOC\_vvv\_nnn\_ddddd.xls* and *ISSBIOC\_vvv\_nnn\_ddddd.sdf***

**Substance ID:** Identification Code;

**ChemName:** Chemical Name;

**CAS:** Registry Number of the Chemical Abstract Service of the chemical;

**Structure:** Chemical Structure;

**Reference:** Source of carcinogenicity data:

**AcToR** (Aggregated Computational Toxicology Resource, <http://actor.epa.gov/actor/faces/ACToRHome.jsp>);

**Circa** (Communication and Information Resource Centre for Administrations, [http://circa.europa.eu/Public/irc/env/bio\\_reports/library?l=/review\\_programme/ca\\_reports&vm=detailed&sb=Title](http://circa.europa.eu/Public/irc/env/bio_reports/library?l=/review_programme/ca_reports&vm=detailed&sb=Title)), Product Type number and year are also provided;

**CPDB** (Carcinogenic Potency Database, <http://potency.berkeley.edu/cpdb.html>);

**FAN Pesticide Project** (Fluoride Action Network, <http://www.fluoridealert.org/researchers/pesticide/>);

**IARC** database (International Agency for Research on Cancer, <http://www.iarc.fr/en/publications/pdfs-online/index.php>);

**ISSCAN\_v4a** (long-term carcinogenicity on rodents database, <http://www.iss.it/ampp/dati/cont.php?id=233&lang=1&tipo=7>);

**NTP** (National Toxicology Program, <http://ntp.niehs.nih.gov/>), the Technical Report number is also provided;

**Toxnet** (database CCRIS from the cluster of toxicological databases Toxnet, <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?CCRIS>).

**FW:** Molecular Weight;

**Formula:** Chemical Formula;

**SMILES:** Simplified chemical notation that represents a chemical structure as a linear textual string. It is aimed at computer applications (for more information, see [http://www.daylight.com/smiles/f\\_smiles.html](http://www.daylight.com/smiles/f_smiles.html));

**Rat\_Male\_Canc; Rat\_Female\_Canc; Mouse\_Male\_Canc; Mouse\_Female\_Canc:**

Carcinogenicity results in the four experimental groups most commonly used for the cancer bioassay: 3 = carcinogen; 2 = equivocal; 1 = noncarcinogen; ND = No Data.

**Overall\_Canc:** Summary carcinogenicity data: 3 = carcinogen; 2 = equivocal; 1 = noncarcinogen. Code 3 is given to chemicals carcinogenic in at least one experimental group; Code 2 is given to chemicals with equivocal results in at least one experimental group, together with negative results in the other experimental groups;

**Overall\_STY:** Overall mutagenicity *in vitro* in *Salmonella typhimurium* (Ames test) from the ISSSTY\_v1a database); ND = No Data.

**Product-Type:** Biocidal product-type (PT) according the Biocides Directive 98/8/EC;

PT can vary from 1 to 23, characterizing the purpose(s) for which the product is to be used.

**Use type:** The specific type of use for the chemical, *e.g.* for pesticides according to the type of pest they control (insecticide, herbicide, fungicide, acaricide etc). This field is not reported for substances with a defined PT.

**Inclusion Directive:** European directive for inclusion of substances in Annex I or IA of Directive 98/8/EC, concerning the placing of biocidal products on the market.