## 2.1. General chemical status information

| Descriptors and registration | |
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| **Parameter** | **Explanation** |
| Reference code | Additional name for the chemical, including those used during substance development and prior to formal naming. |
| Alias's/synonyms (below the substance name) | Other names by which the substance is known. These are enabled in the various database search facilities. |
| Summary | This is a short paragraph picking out the key parameters providing an overview of the pesticide substance and it chemical and (eco)toxicological properties. |
| Data alerts | These alerts are based on data in the tables discussed below to highlight areas of potential concern. However, the absence of an alert does not imply that a substance has no implications for human health, biodiversity or the environment, just that we do not have the data to form a judgement. |
| Description | General description of the major uses of the substance. |
| Example pests controlled | A non-exhaustive list of pests that the substance controls. |
| Example applications | A non-exhaustive list of application situations. |
| Efficacy & activity | Information on the efficacy and activity of the pesticide towards the pest or issue the substance is intended to control. |
| Appearance and life cycle (BPDB only) | A brief description of the form taken by the organism and the key elements of its life cycle. |
| Availability status | An indication of whether the substance is currently available or obsolete (if known). |
| Introduction & key dates | Various key dates in the substance's history such as the date of discovery, patents, product launches, regulatory approval, withdrawal etc. |
| Taxonomic classification (BPDB only) | Taxonomic classification of the organism. |
| Examples of species treated (VSDB only) | Key livestock types for which the substance is used as a veterinary product. |
| UK regulatory status (PPDB/BPDB only) | Status of the chemical within UK approvals system. |
| EC Regulation 1107/2009 status (PPDB/BPDB only) | Status of the chemical in the EU peer review process EC directive 1107/2009 (repealing 91/414) of pesticide/biopesticide active substances. |
| Dossier rapporteur/co-rapporteur (PPDB/BPDB only) | National regulatory authority responsible for regulatory assessment. |
| Date EC 1107/2009 inclusion expires (PPDB/BPDB only) | Date current EU status expires (if appropriate). |

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| EU Candidate for substitution (CfS) (PPDB/BPDB only) | These are pesticide active substances identified during the EU regulatory assessment process as having a less favourable toxicological or environmental profile but which still satisfy the criteria for approval. The criteria for selection includes (for example) substances which are carcinogenic, those which have negative effects on reproduction and those that are a high risk to groundwater whilst also showing a toxic effect of concern. |
| Listed in EU database (PPDB/BPDB only) | Whether the substance is present in the EU approvals database. |
| Approved for use or known to be used in the following EU-27 Member States (PPDB/BPDB only) | Provides an indication of where the active substance has been authorised for agricultural use within the EU. Please check with the relevant national authority before relying on this data. |
| Also used in / Additional information (PPDB/BPDB only) | Other countries where we believe the substance is used. Please check with the relevant national authority before relying on this data. |

## Chemical structure information

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| Isomerism | This is a description of the isomeric nature of the substance. |
| Chemical formula | This is a concise way of expressing information about the atoms that constitute the chemical. |
| Canonical SMILES | The **S**implified Molecular **I**nput **L**ine **E**ntry **S**pecification (SMILES) is a specification for describing the structure of chemical molecules using short ASCII strings. SMILES strings can be imported by most molecule editors for conversion back into drawings or models of the molecules. Canonical SMILES are those used by the most common applications and omits isotopic and chiral information. |
| Isomeric SMILES | SMILES as above but including isotopic and chiral information. |
| International Chemical Identifier key (InChIKey) | IUPAC **In**ternational **Ch**emical **I**dentifier. This is a textual identification for chemical substances, that provides a standard, readable way of encoding molecular information and to facilitate the search for such information in databases and on the web. This parameter is a condensed version of the InChI Identified described below. |
| International Chemical Identifier (InChI) | IUPAC **In**ternational **Ch**emical **I**dentifier. This is a textual identification for chemical substances, that provides a standard, readable way of encoding molecular information and to facilitate the search for such information in databases and on the web. |
| CAS RN | Chemical Abstracts Service Registry Number - a unique identify for the chemical. |
| Alternative/old CAS RN | Additional/old Chemical Abstracts Service Registry Number(s) for the substance. |
| EC number | The unique reference number for the chemical in the European Chemical Substances Information System (EINECS) or European List of Notified Chemicals (ELINCS). |

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| CIPAC number | The CIPAC code number system is a simple approach for an unambiguous coding of chemicals. CIPAC, FAO, WHO and the EU are the main users of this system. |
| US EPA chemical code | The U.S. Environmental Protection Agency (U.S. EPA) assigns a unique reference number to individual pesticide active ingredients to assist in their identification. This code is sometimes referred to as the Shaugnessy Number. |
| PubChem CID | Identifier within the PubChem chemistry database of the National Institutes of Health (NIH). |
| 2D structure diagram/image available? | Either Yes or No. If Yes is stated this will be a link to a separate window displaying the structure diagram. |
| 3D structure diagram/image available? (PPDB only) | If appropriate a link will be provided to the Cambridge Crystallographic Data Centre structural 3D diagram page. |

## General information

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| Pesticide, biopesticide or veterinary substance type | The specific type of substance described according to the type of pest or disease they control e.g. Insecticide, Herbicide, Fungicide, Acaricide, Antiparasitic, Anthelmintic etc. |
| Metabolite type | General description of the host process that creates the metabolite e.g. soil, surface water, animal, plant, groundwater. |
| Other bioactivity and use | General description of any other bioactivity or applications. |
| Substance group | Chemical classification group based on the chemical structure. |
| Minimum active substance purity | Minimum substance purity of the active ingredient. |
| Known relevant impurities | Information on any relevant impurities declared for the substance. |
| Substance origin | Whether the substance is natural or synthetic. |
| Mode of action | The mechanism by which the substance performs its main function. |
| Molecular target (VSDB only) | This is the key molecule involved in a particular metabolic or signalling pathway that is specific to the disease condition or pathology or to the infectivity or survival of a microbial pathogen. |
| Substance source (BPDB only) | The origin of the organism/substance. |
| Substance production (BPDB only) | How the organism/substance is produced. |
| Uses (BPDB only) | What the organism/substance is used for. |
| Target pests (BPDB only) | What pests the organism/substance can be used to treat. |
| Target host (BPDB only) | What crops the organism/substance can be used in. |

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| Farming system suitability (BPDB only) | Comments of the suitability of the organism/substance for use in different farming systems. |
| ATCvet Code (VSDB only) | The WHO's Anatomical Therapeutic Chemical Classification System for veterinary medicinal products (ATCvet) is used to classify veterinary drugs. |
| Therapeutic Class (VSDB only) | The broad therapeutic grouping of the substance. |
| Controlled Drug? (VSDB only) | Whether the substance is a controlled drug or not under UK legislation. |
| Regulation 37/2010 MRL Classification (VSDB only) | EU Regulation 37/2010 classifies pharmacologically active substances according to their permitted maximum residue limits in food of animal origin. |
| Molecular mass | The relative molecular mass (molecular weight) of a chemical is the mass of a molecule of the chemical relative to the mass of a carbon atom taken as exactly 12. |
| Chemical name | Name of the chemical according to the nomenclature rules of IUPAC or CAS. Where this is not available or does not apply a generic name is given. |
| Forever chemicals | 'Forever chemicals' refers to per- and polyfluoroalkyl substances (PFAS), a group of synthetic chemicals known for their extreme persistence in the environment along with their, often, harmful effects on human health. Within the PPDB substances are classified as PFAS under one or more of the following definitions:<br>a) the OECD,<br>b) one or both of the definitions adopted by the USEPA,<br>c) the EU.<br>**The OECD Definition (2021)** is the most inclusive definition and states that PFAS are fluorinated substances that contain at least one fully fluorinated methyl (–$CF_3$) or methylene (–$CF_2$–) carbon atom, with no hydrogen, chlorine, bromine, or iodine attached.<br>**The two US EPA definitions** are:<br>• TSCA (Toxic Substances Control Act): Defines PFAS based on specific structural units like R–$CF_2$–CF(R')(R"), where none of the R groups are hydrogen.<br>• CCL5 (Drinking Water Contaminant Candidate List): Includes chemicals with one of three specific fluorinated structures, making it less inclusive than OECD but broader than TSCA.<br>**The EU definition offered by the European Chemicals Agency (ECHA)** includes any substance with at least one fully fluorinated methyl or methylene group |
| Highly Hazardous Pesticide (HHP; Type I & Type II) | There are many ways in which a chemical may be classified for the hazards it poses to humans and the environment. As well as the PPDB's traffic light system we have two classifications for 'Highly Hazardous Pesticides' (HHPs):<br>The aim of these HHP classifications is to promote global phase-outs, support safer alternatives, and protect vulnerable populations, workers, and ecosystems from harmful exposures.<br>• Note: if a substance does not have an HHP classification, it does not necessarily mean Type I is primarily based on the hazards it poses to human |

health via oral or dermal exposure and uses a high toxicity threshold. This is based on the approach and criteria established by the FAO/WHO Joint Meeting on Pesticide Management (JMPM) and further details can be found here. The classification herein is based entirely on PPDB data for transparency. Note that Criterion 8 is not used as it is bespoke to each country.

- Type II is broader than Type I taking into account human health impacts from exposure due to inhalation, has a slightly lower toxicity threshold and includes environmental impacts, specifically aquatic and honey bee toxicity, environmental persistence and bioaccumulation. The rules applied (criteria) are closely aligned to those used by PAN (Pesticide Action Network). Again the classifications, herein are based wholly on PPDB data.

No HHP classification does not, necessarily, mean the substance is not highly hazardous, as it maybe that there is insufficient information to make an assessment.

**Type I HHPs**

This is based on the criteria adopted by the Food and Agriculture Organization of the United Nations and World Health Organization (FAO & WHO, 2016); however, the HHP classification given here is wholly determined from data within the PPDB, and may not necessarily be identical to the HPP classifications produced by other data providers, who may not be using the same data. In the PPDB this is determined using:

- **Criterion 1:** Pesticide active ingredients that meet the criteria of classes Ia or Ib of the WHO Recommended Classification of Pesticides by Hazard – see 'WHO classification' below.
- **Criterion 2:** Pesticide active ingredients that meet the criteria of carcinogenicity Categories 1A and 1B of the Globally Harmonized System on Classification and Labelling of Chemicals (GHS) – those with a CLP classification of H350 (see 'CLP classification' below).
- **Criterion 3:** Pesticide active ingredients that meet the criteria of mutagenicity Categories 1A and 1B of the Globally Harmonized System on Classification and Labelling of Chemicals (GHS) – those with a CLP classification of H340 (see 'CLP classification' below).
- **Criterion 4:** Pesticide active ingredients that meet the criteria of reproductive toxicity Categories 1A and 1B of the Globally Harmonized System on Classification and Labelling of Chemicals (GHS) – those with a CLP classification of H360 (see 'CLP classification' below).
- **Criterion 5:** Pesticide active ingredients listed by the Stockholm Convention in its Annexes A and B, and those meeting all the criteria in paragraph 1 of Annex D of the Convention – those identified as Persistent Organic Pollutants (POPs) in annexes A or B of the Stockholm Convention (see 'Other status information' below).
- **Criterion 6:** Pesticide active ingredients listed by the Rotterdam Convention in its Annex III – those subject to PIC (Prior Informed Consent) regulations under the Rotterdam Convention (see 'Other status information' below).
- **Criterion 7:** Pesticides listed under the Montreal Protocol – those identified as substances that deplete the ozone layer under the Montreal Protocol (see 'Other status information' below).

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| | • **Criterion 8:** Pesticide active ingredients that have shown a high incidence of severe or irreversible adverse effects on human health or the environment - Not used in the PPDB.<br><br>**Type II HHPs**<br>Pesticide active substances have been identified as Type II HHPs if they meet one or more of the following criteria. Pesticide active substances that:<br>1. Meet the criteria of classes Ia or Ib of the WHO Recommended Classification of Pesticides by Hazard (or those with a CLP classification of H330)<br>2. Meet the criteria of carcinogenicity Categories 1A and 1B of the Globally Harmonized System on Classification and Labelling of Chemicals (GHS) (those with a CLP classification of H350)<br>3. Meet the criteria of mutagenicity Categories 1A and 1B of the Globally Harmonized System on Classification and Labelling of Chemicals (GHS) (those with a CLP classification of H340)<br>4. Meet the criteria of reproductive toxicity Categories 1A and 1B of the Globally Harmonized System on Classification and Labelling of Chemicals (GHS) (those with a CLP classification of H360)<br>5. Are confirmed endocrine disruptors according to the World Health Organization (WHO) definition of an endocrine disruptor<br>6. Are listed by the Stockholm Convention in its Annexes A and B, and those meeting all the criteria in paragraph 1 of Annex D of the Convention (those identified as Persistent Organic Pollutants (POPs) in annexes A or B of the Stockholm Convention)<br>7. Are listed by the Rotterdam Convention in its Annex III (those subject to PIC (Prior Informed Consent) regulations under the Convention)<br>8. Are listed under the Montreal Protocol (those identified as substances that deplete the ozone layer under the Protocol)<br>9. Have demonstrated a high aquatic toxicity (where acute ecotoxicity for fish, invertebrates or algae =< 0.1 mg $l^{-1}$)<br>10. Have demonstrated a high toxicity to bees (where contact or oral bee toxicity =< 2 µg $bee^{-1}$)<br>11. Are environmentally persistent (where sediment phase only $DT_{50}$ => 90 days or water phase only $DT_{50}$ => 90 days or $DT_{50}$ (field) => 60 days (or, where $DT_{50}$ (field) is not available, where $DT_{50}$ (lab) => 60 days))<br>12. Are bioaccumulative (where bio-concentration factor (BCF) > 2000 l $kg^{-1}$ (or, if BCF is not available, where Log P >=5))<br>The Type II HHP classification given here is determined from the data wholly within the PPDB. It may not, necessarily, be identical to the HPP classifications produced by other data providers who may not be using the same data. |
| UK Poisons List Order 1972 | The UK Poisons Order 1972 regulates the sale, supply, and handling of hazardous chemicals classified as poisons. Hazardous substances to which this regulation apply are listed in annex's. More information at: https://www.legislation.gov.uk/uksi/1972/1938/resources. |
| Rotterdam Convention (PIC Regulations) | The Rotterdam Convention and PIC Regulations aim to ensure safe international trade of hazardous chemicals and pesticides through shared responsibility and transparency. The Convention establishes a Prior Informed |

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| | Consent (PIC) procedure, requiring countries to be notified and give explicit consent before certain hazardous chemicals are exported to them. This helps protect human health and the environment by ensuring importing countries have the necessary information to manage risks. More information at: https://www.pic.int/en-us/procedures/picprocedure.aspx. |
| Montreal Protocol | The Montreal Protocol is a global treaty designed to protect the ozone layer by phasing out the production and use of ozone-depleting substances. More information at: https://www.unep.org/ozonaction/who-we-are/about-montreal-protocol. |
| Stockholm Convention (Persistent Organic Pollutant) | The Stockholm Convention is a global treaty aimed at protecting human health and the environment from persistent organic pollutants (POPs). More information at: https://www.pops.int/. |
| OSPAR listed marine pollutant | OSPAR is a regional convention that protects the marine environment of the North-East Atlantic through international cooperation. The Convention identifies hazardous substances that pose a threat to the North-East Atlantic marine environment. These substances are categorized into several sections within the List of Substances of Possible Concern (LSPC) and the List of Chemicals for Priority Action, which guide monitoring, regulation, and elimination efforts. See also: https://www.ospar.org/work-areas/hasec/hazardous-substances. |
| EU Water Framework Directive listed substance | The EU Water Framework Directive (WFD) substance list identifies pollutants that pose significant risks to aquatic environments and sets strict controls to monitor and reduce their presence. |
| Other status information | This will display information relating to the status of the substance with respect to other legislation, international conventions and information regarding phase out. Including:<br>**LRTAP Chemicals:** The Convention on Long-range Transboundary Air Pollution (LRTAP): The aim of the Convention is that Parties seek to limit and, as far as possible, gradually reduce and prevent air pollution including long-range transboundary air pollution. Chemicals considered to be the most serious problem are assigned to Annex 1.<br>**PAN Dirty Dozen / PAN Bad Actor:** The Pesticide Action Network (PAN) have identified these chemicals as being particularly harmful.<br>**Environmental contaminant:** substance is known to have polluted groundwaters, surface waters or other environmental media and is a substance of concern. |
| Relevant environmental water quality standards | This field gives an indication of the quality standards in place for the protection of aquatic life. |
| Resistance code (HRAC, WSSA, IRAC, FRAC) (PPDB/BPDB only) | This is the HRAC, WSSA, IRAC or FRAC code that denotes their resistance classification and can be used in resistance management programmes. |
| Examples of recorded resistance | Information on any known resistance issues for the substance. |

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| Physical state | Provides an indication of the physical state of the material – solid, liquid or gas and its general appearance. This normally applies to the active substance in its pure state unless stated otherwise. |
| Related substances & organisms (BPDB only) | Any known related substances and organisms and links to their pages if appropriate. |
| Can be a metabolite of | Information on the substances of which the relevant substance can be a metabolite and links to their pages if appropriate. |