

2.1. General chemical status information

Descriptors and registration	
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 its 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).
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

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 M olecular I nterpretation L ine E nter 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 I nternational C hemical 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 I nternational C hemical 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).
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 Shaughnessy 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

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.
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.
Other status information	<p>This will display information relating to the status of the substance with respect to other legislation, international conventions and information regarding phase out. Including:</p> <p>PIC Annex 1 chemicals: The Rotterdam Convention on Prior Informed Consent (PIC). The Convention covers pesticides and industrial chemicals that have been banned or severely restricted for health or environmental reasons by parties and which have been notified for inclusion in the PIC procedure by those parties.</p> <p>POP chemicals: The Stockholm Convention on Persistent Organic Pollutants (POPs). The Stockholm Convention bans or severely restricts the most hazardous POPs, and establishes an international, science-based process for adding other POPs to the treaty. Those listed in this database also include chemicals that are new POP candidates proposed by other organisations including the WWF.</p> <p>VOC chemicals: Volatile organic compounds (VOCs) are organic chemical compounds that have high enough vapour pressures under normal conditions to significantly vaporise and enter the atmosphere.</p> <p>The term VOC may have special legal meanings in some countries.</p> <p>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.</p> <p>PAN Dirty Dozen / PAN Bad Actor: The Pesticide Action Network (PAN) have identified these chemicals as being particularly harmful.</p>

	<p>OSPAR: OSPAR Convention for the Protection of the Marine Environment: pfa - priority substances for action, soc - substances of concern.</p> <p>WFD: Water Framework Directive 2000/60/EC: phs - priority hazardous substance, pps - possible priority substance, other - other substance of concern.</p> <p>Groundwater contaminant: substance is known to have polluted groundwaters and is a substance of concern.</p>
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.
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.