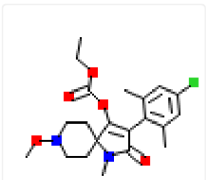
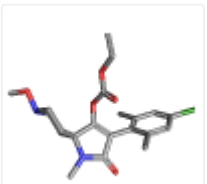
PubChem

COMPOUND SUMMARY

Elestal

PubChem CID	58537978
Structure	 2D  3D Find Similar Structures
Chemical Safety	 Irritant  Environmental Hazard Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_{21}H_{27}ClN_2O_5$
Synonyms	Spiropidion UNII-ZVZ9ZYT899 ZVZ9ZYT899 1229023-00-0 Elestal More...
Molecular Weight	422.9
Dates	Modify 2022-08-27 Create 2012-08-19

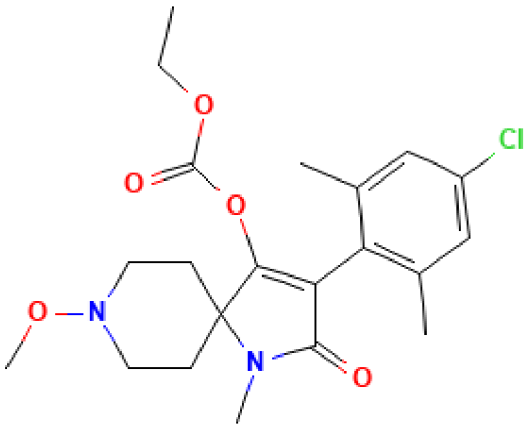
Spiropidion is an azaspiro compound that is 1-methoxypiperidine which is fused at position 4 to the 5-position of a 1,5-dihydro-2H-pyrrol-2-one that is substituted at positions 1, 3 and 4 by methyl, 4-chloro-2,6-dimethylphenyl and (ethoxycarbonyl)oxy groups, respectively. It is a proinsecticide developed by Syngenta and used to protect a wide range of crops from some of the most damaging, difficult to control sucking pests such as aphids, whiteflies, Pysllids, armoured scales, soft scales, spider mites, rust mites, and red mites including California red scale, green peach aphid (Myzus persicae), tobacco whitefly etc. It has a role as an EC 6.4.1.2 (acetyl-CoA carboxylase) inhibitor, a proinsecticide and an agrochemical. It is a member of tetramic acids, a member of monochlorobenzenes, an azaspiro compound and a carbonate ester.

▸ ChEBI

1 Structures

1.1 2D Structure

Chemical Structure Depiction



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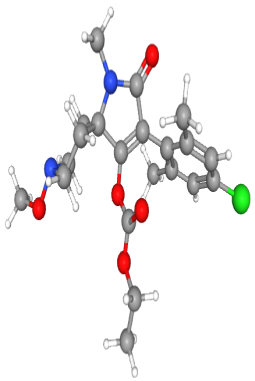
1.2 3D Conformer

Interactive Chemical Structure Model

- Ball and Stick
- Sticks
- Wire-Frame
- Space-Filling
- Show Hydrogens
- Animate



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2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

[3-(4-chloro-2,6-dimethylphenyl)-8-methoxy-1-methyl-2-oxo-1,8-diazaspiro[4.5]dec-3-en-4-yl] ethyl carbonate

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

PubChem

2.1.2 InChI

InChI=1S/C21H27ClN2O5/c1-6-28-20(26)29-18-17(16-13(2)11-15(22)12-14(16)3)19(25)23(4)21(18)7-9-24(27-5)10-8-21/h11-12H,6-10H2,1-5H3

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

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2.1.3 InChIKey

WOPFPAIGRGHWAQ-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

2.1.4 Canonical SMILES

CCOC(=O)OC1=C(C(=O)N(C12CCN(CC2)OC)C)C3=C(C=C(C=C3C)Cl)C

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.2 Molecular Formula

C21H27ClN2O5

Computed by PubChem 2.1 (PubChem release 2021.05.07)

PubChem

2.3 Other Identifiers

2.3.1 CAS

1229023-00-0

ChemIDplus; European Chemicals Agency (ECHA)

2.3.2 European Community (EC) Number

815-785-2

European Chemicals Agency (ECHA)

2.3.3 UNII

ZVZ9ZYT899

FDA/SPL Indexing Data

2.3.4 Wikidata

Q106030544

Wikidata

2.4 Synonyms

2.4.1 Depositor-Supplied Synonyms

Spiropidion
UNII-ZVZ9ZYT899
ZVZ9ZYT899
1229023-00-0
Elestal
3-(4-Chloro-2,6-dimethylphenyl)-8-methoxy-1-methyl-2-oxo-1,8-diazaspiro(4.5)dec-3-en-4-yl ethyl carbonate
3-(4-chloro-2,6-dimethylphenyl)-8-methoxy-1-methyl-2-oxo-1,8-diazaspiro[4.5]dec-3-en-4-yl ethyl carbonate
Spiropidion [ISO]
SCHEMBL46202
CHEBI:167159
SYN546330
3-(4-chloro-2,6-xylyl)-8-methoxy-1-methyl-2-oxo-1,8-diazaspiro[4.5]dec-3-en-4-yl ethyl carbonate

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3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	422.9	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	3.5	Computed by XLogP3 3.0 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	6	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Rotatable Bond Count	6	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	422.1608497	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	422.1608497	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	68.3 Å²	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	29	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	662	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.05.07)

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4 Related Records

4.1 Related Compounds with Annotation

PubChem

4.2 Related Compounds

Mixtures, Components, and Neutralized Forms	4 Records
Similar Compounds	66 Records
Similar Conformers	327 Records

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4.3 Substances

4.3.1 Related Substances

All	14 Records
Same	10 Records
Mixture	4 Records

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4.3.2 Substances by Category

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5 Safety and Hazards

5.1 Hazards Identification

5.1.1 GHS Classification

Pictogram(s)	 Irritant  Environmental Hazard
Signal	Warning
GHS Hazard Statements	H317 (100%): May cause an allergic skin reaction [Warning Sensitization, Skin] H332 (100%): Harmful if inhaled [Warning Acute toxicity, inhalation] H410 (100%): Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]
Precautionary Statement Codes	P261, P271, P272, P273, P280, P302+P352, P304+P340, P317, P321, P333+P313, P362+P364, P391, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*The GHS information provided by 1 company from 1 notification to the ECHA C&L Inventory.*

▶ European Chemicals Agency (ECHA)

5.1.2 Hazard Classes and Categories

Skin Sens. 1 (100%)

Acute Tox. 4 (100%)

Aquatic Chronic 1 (100%)

▶ European Chemicals Agency (ECHA)

6 Literature

6.1 Chemical Co-Occurrences in Literature

PubChem

7 Patents

7.1 Depositor-Supplied Patent Identifiers

PubChem

Link to all deposited patent identifiers

PubChem

7.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=WOPFPAIGRGHWAQ-UHFFFAOYSA-N

PATENTSCOPE (WIPO)

8 Classification

8.1 ChEBI Ontology

ChEBI

8.2 ChemIDplus

ChemIDplus

8.3 UN GHS Classification

UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

9 Information Sources

FILTER BY SOURCE ALL SOURCES

1. ChEBI

Spiropidion
http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:167159

ChEBI Ontology
http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology

2. ChemIDplus

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https://www.nlm.nih.gov/copyright.html

Spiropidion [ISO]
https://chem.nlm.nih.gov/chemidplus/sid/1229023000

ChemIDplus Chemical Information Classification
https://chem.nlm.nih.gov/chemidplus/

3. European Chemicals Agency (ECHA)

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[2-(4-chloro-2,6-dimethyl-phenyl)-8-methoxy-4-methyl-3 oxo-4,8-diazaspiro[4,5]dec-1-en-1-yl] ethyl carbonate
https://echa.europa.eu/information-on-chemicals

[2-(4-chloro-2,6-dimethyl-phenyl)-8-methoxy-4-methyl-3 oxo-4,8-diazaspiro[4,5]dec-1-en-1-yl] ethyl carbonate
https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/257587

4. FDA/SPL Indexing Data

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ZVZ9ZYT899
https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/

5. Wikidata

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spiropidion
https://www.wikidata.org/wiki/Q106030544

6. PubChem
https://pubchem.ncbi.nlm.nih.gov

7. UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

GHS Classification Tree
http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

8. PATENTSCOPE (WIPO)

SID 392812842
https://pubchem.ncbi.nlm.nih.gov/substance/392812842