

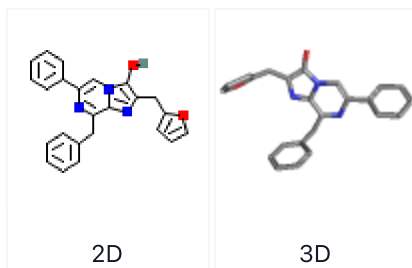
COMPOUND SUMMARY

Furimazine

PubChem CID

136008305

Structure



2D

3D

Chemical Safety



Irritant

[Laboratory Chemical Safety Summary \(LCSS\) Datasheet](#)

Molecular Formula

C₂₄H₁₉N₃O₂

Synonyms

Furimazine
1374040-24-0
8-benzyl-2-(furan-2-ylmethyl)-6-phenylimidazo[1,2-a]pyrazin-3(7H)-one
8-Benzyl-2-[(furan-2-yl)methyl]-6-phenylimidazo[1,2-a]pyrazin-3(7H)-one
8-benzyl-2-(furan-2-ylmethyl)-6-phenylimidazo[1,2-a]pyrazin-3-ol

[View More...](#)

Molecular Weight

381.4 g/mol

Computed by PubChem 2.2 (PubChem release 2021.10.14)

Dates

Create: Modify:
2019-01-21 2024-11-09

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5 Chemical Vendors	
6 Pharmacology and Biochemistry	▼
7 Safety and Hazards	▼
8 Literature	▼
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1 Structures

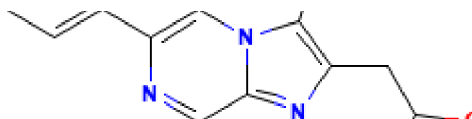


1.1 2D Structure






Chemical Structure Depiction

The image shows a chemical structure viewer interface. On the left, there is a label 'Chemical Structure Depiction'. The main area displays the 2D chemical structure of Furimazine, which is a 1,2,3,4-tetrahydronaphthalene derivative with a 1H-imidazole ring fused at the 1-position. The structure is shown in a skeletal format with a red oxygen atom and a green hydrogen atom attached to the imidazole ring. At the bottom, there is a small icon of the structure and a plus sign in a box. The top right corner of the viewer has search, image, and download icons.

[► PubChem](#)

1.2 3D Conformer








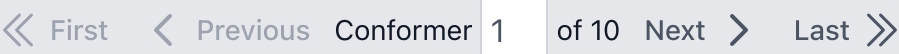
Interactive Chemical Structure Model

☒ Ball and Stick ☐ Sticks ☐ Wire-Frame ☐ Space-Filling

☒ Show Hydrogens ☐ Animate





[► PubChem](#)

2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



8-benzyl-2-(furan-2-ylmethyl)-6-phenylimidazo[1,2-a]pyrazin-3-ol

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

► [PubChem](#)

2.1.2 InChI



InChI=1S/C₂₄H₁₉N₃O₂/c28-24-21(15-19-12-7-13-29-19)26-23-20(14-17-8-3-1-4-9-17)25-22(16-27(23)24)18-10-5-2-6-11-18/h1-13,16,28H,14-15H2

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

► [PubChem](#)

2.1.3 InChIKey



HTBLMRUZSCCOLL-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

► [PubChem](#)

2.1.4 SMILES



C1=CC=C(C=C1)CC2=NC(=CN3C2=NC(=C3O)CC4=CC=CO4)C5=CC=CC=C5

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

► [PubChem](#)

2.2 Molecular Formula



C₂₄H₁₉N₃O₂

Computed by PubChem 2.2 (PubChem release 2021.10.14)

► [PubChem](#)

2.3 Other Identifiers



2.3.1 CAS



1374040-24-0

- ▶ European Chemicals Agency (ECHA)

2.3.2 European Community (EC) Number



846-449-3

- ▶ European Chemicals Agency (ECHA)

2.3.3 Nikkaji Number



J3.661.436F

- ▶ Japan Chemical Substance Dictionary (Nikkaji)

2.4 Synonyms



2.4.1 MeSH Entry Terms



8-Benzyl-2-(2-furylmethyl)-6-phenylimidazo(1,2-a)pyrazin-3(7H)-one
furimazine
hydrofurimazine

- ▶ Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms



Furimazine	PBI 3939
1374040-24-0	MFCD31657402
8-benzyl-2-(furan-2-ylmethyl)-6-phenylimidazo[1,2-a]pyrazin-3(7H)-one	AKOS040741773
8-Benzyl-2-[(furan-2-yl)methyl]-6-phenylimidazo[1,2-a]pyrazin-3(7H)-one	AT42004
8-benzyl-2-(furan-2-ylmethyl)-6-phenylimidazo[1,2-a]pyrazin-3-ol	AC-33265
8-benzyl-2-[(furan-2-yl)methyl]-6-phenyl-3H,7H-imidazo[1,2-a]pyrazin-3-one	DA-63640
Furimazine?	HY-111497
SCHEMBL2670126	CS-0042265
BUFSEVFXVCFYKY-UHFFFAOYSA-N	8-benzyl-2-(furan
GLXC-15618	

[EX-A5736](#)[► PubChem](#)

3 Chemical and Physical Properties



3.1 Computed Properties



Property Name	Property Value	Reference
Molecular Weight	381.4 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
XLogP3-AA	5.3	Computed by XLogP3 3.0 (PubChem release 2021.10.14)
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Hydrogen Bond Acceptor Count	4	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Rotatable Bond Count	5	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Exact Mass	381.147726857 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Monoisotopic Mass	381.147726857 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Topological Polar Surface Area	63.6Å ²	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Heavy Atom Count	29	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	520	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
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 2021.10.14)

► [PubChem](#)

4 Related Records



4.1 Related Compounds with Annotation



Follow these links to [do a live 2D search](#) or [do a live 3D search](#) for this compound, sorted by annotation score. This section is deprecated (see [here](#) for details), but these live search links provide equivalent functionality to the table that was previously shown here.

► [PubChem](#)

4.2 Related Compounds



Same Connectivity Count	2
Same Parent, Connectivity Count	7
Same Parent, Exact Count	6
Mixtures, Components, and Neutralized Forms Count	25
Similar Compounds (2D)	View in PubChem Search

Similar Conformers
(3D)

[View in PubChem Search](#)

► [PubChem](#)

4.3 Substances



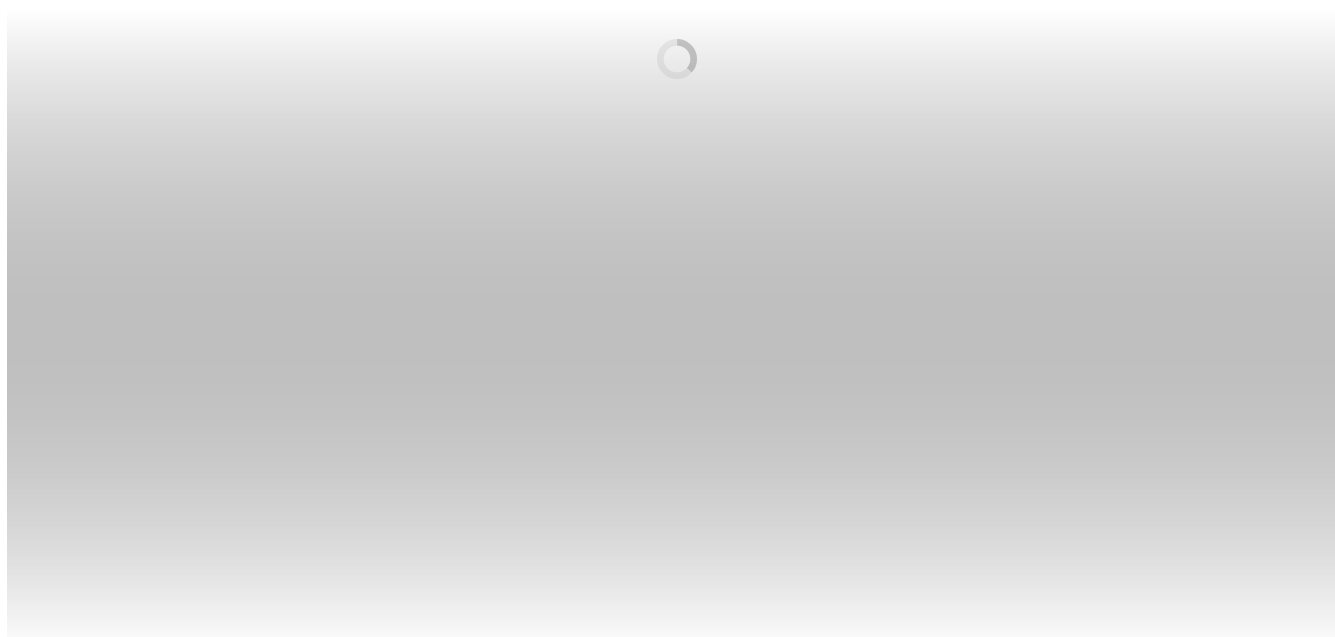
4.3.1 Related Substances



All Count	71
Same Count	46
Mixture Count	25

► [PubChem](#)

4.3.2 Substances by Category



► [PubChem](#)

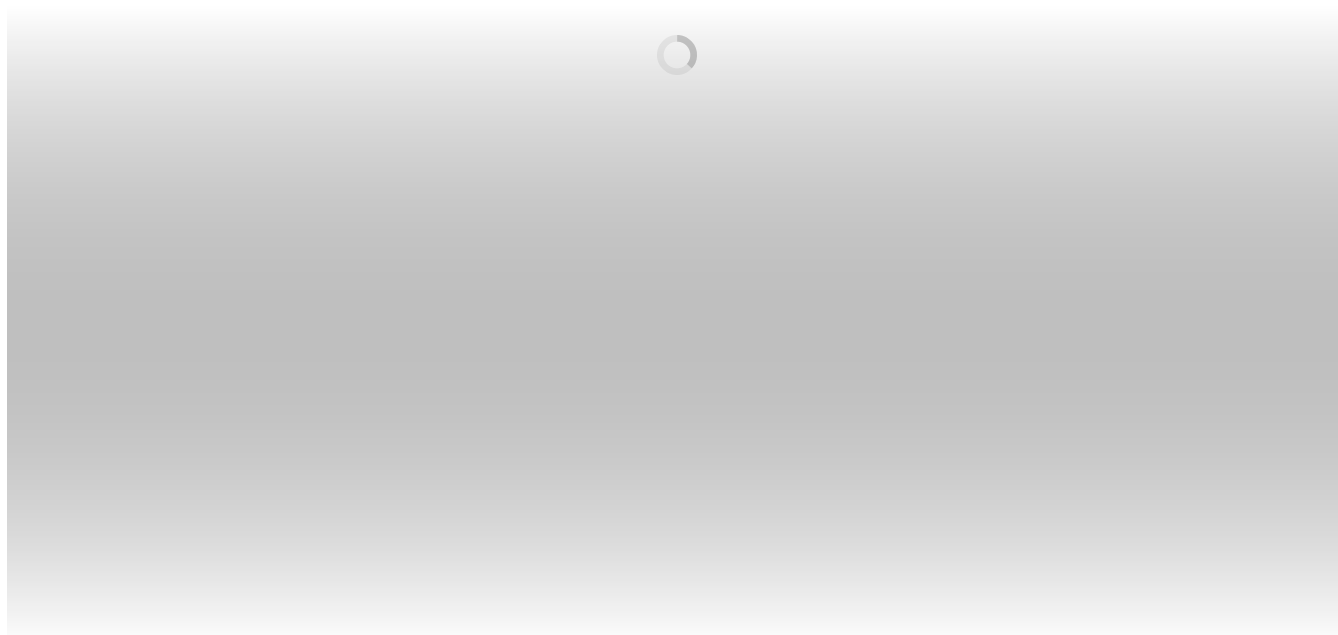
4.4 Entrez Crosslinks



PubMed Count	1
--------------	---

[► PubChem](#)

5 Chemical Vendors

[► PubChem](#)

6 Pharmacology and Biochemistry



6.1 MeSH Pharmacological Classification



Luminescent Agents

Compound such as LUMINESCENT PROTEINS that cause or emit light (PHYSICAL LUMINESCENCE). (See [all compounds classified as Luminescent Agents.](#))

[► Medical Subject Headings \(MeSH\)](#)

7 Safety and Hazards




7.1 Hazards Identification



7.1.1 GHS Classification



Pictogram(s)	 <p>Irritant</p>
Signal	Warning
GHS Hazard Statements	<p>H302 (100%): Harmful if swallowed [Warning Acute toxicity, oral]</p> <p>H315 (100%): Causes skin irritation [Warning Skin corrosion/irritation]</p> <p>H319 (100%): Causes serious eye irritation [Warning Serious eye damage/eye irritation]</p> <p>H335 (100%): May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation]</p>
Precautionary Statement Codes	<p>P261, P264, P264+P265, P270, P271, P280, P301+P317, P302+P352, P304+P340, P305+P351+P338, P319, P321, P330, P332+P317, P337+P317, P362+P364, P403+P233, P405, and P501</p> <p>(The corresponding statement to each P-code can be found at the GHS Classification page.)</p>
ECHA C&L Notifications Summary	<i>The GHS information provided by 1 company from 1 notification to the ECHA C&L Inventory.</i>

► [European Chemicals Agency \(ECHA\)](#)

7.1.2 Hazard Classes and Categories



Acute Tox. 4 (100%)

Skin Irrit. 2 (100%)

Eye Irrit. 2A (100%)

STOT SE 3 (100%)

► [European Chemicals Agency \(ECHA\)](#)

8 Literature



8.1 Consolidated References





► PubChem

8.2 NLM Curated PubMed Citations



► PubChem

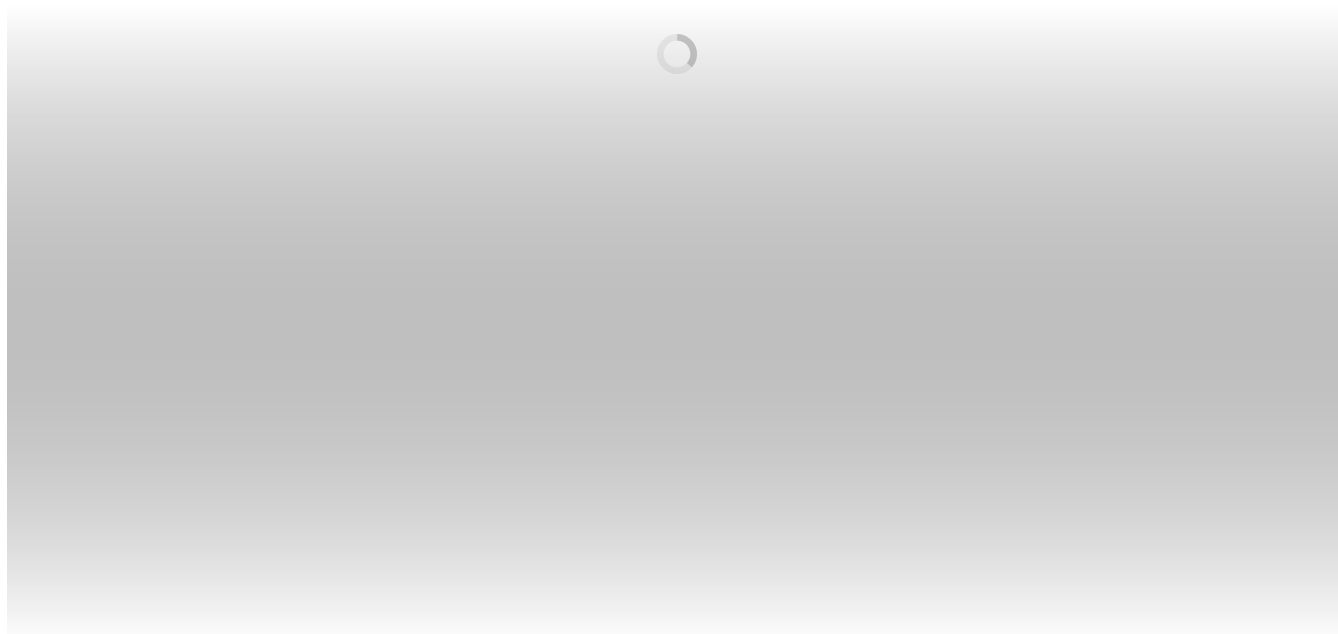
8.3 Nature Journal References



Su et al. An optimized bioluminescent substrate for non-invasive imaging in the brain. Nature Chemical Biology, DOI: 10.1038/s41589-023-01265-x, published online 9 February 2023

► Nature Chemical Biology

8.4 Chemical Co-Occurrences in Literature



► PubChem

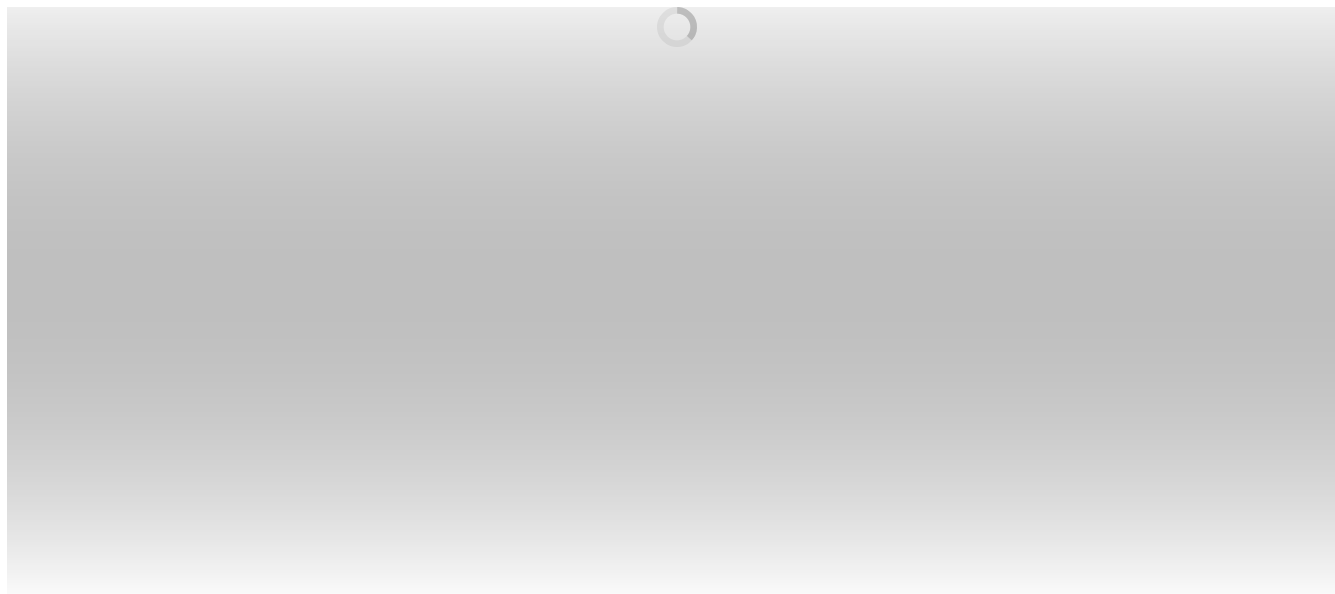
8.5 Chemical-Gene Co-Occurrences in Literature



► PubChem

8.6 Chemical-Disease Co-Occurrences in Literature



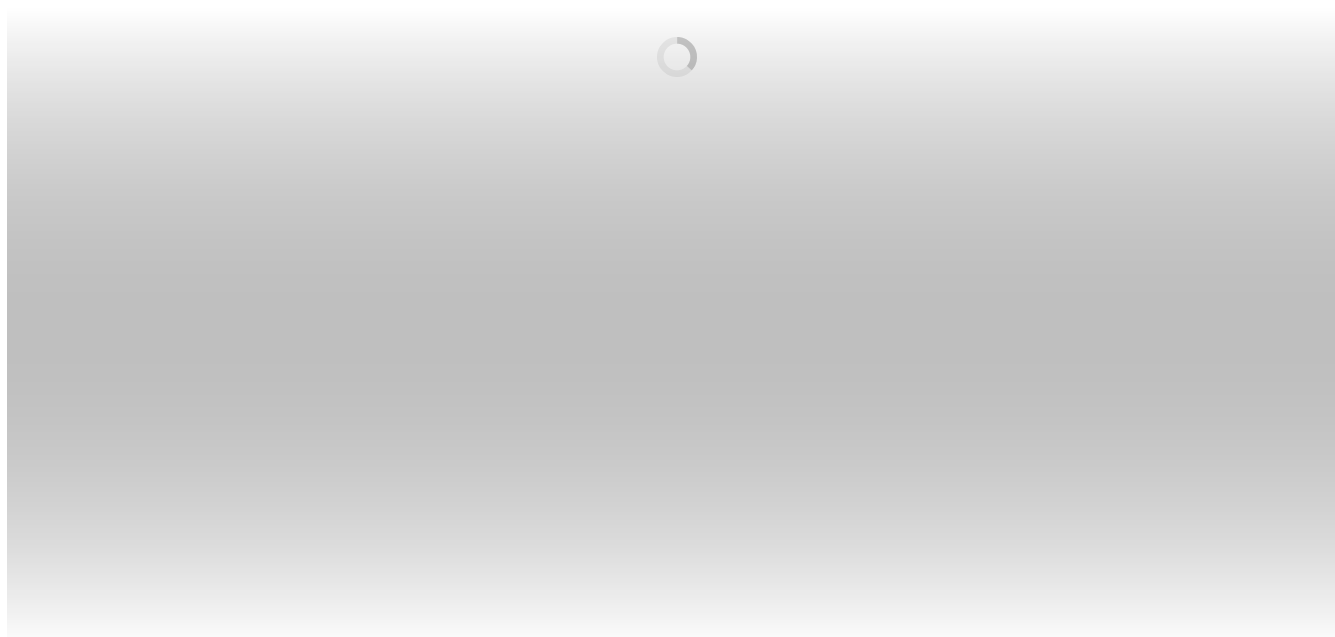


► PubChem

9 Patents



9.1 Depositor-Supplied Patent Identifiers



► PubChem

[Link to all deposited patent identifiers](#)

► PubChem

9.2 WIPO PATENTSCOPE

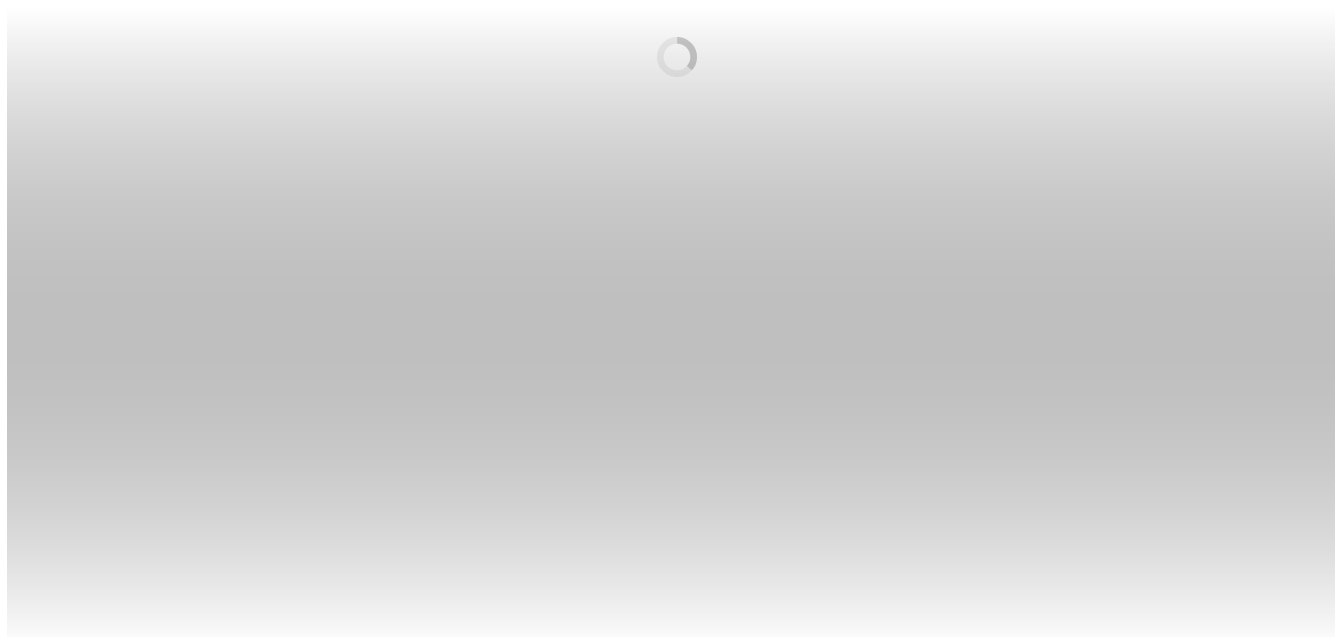


Patents are available for this chemical structure:

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

► PATENTSCOPE (WIPO)

9.3 Chemical Co-Occurrences in Patents



► PubChem

9.4 Chemical-Disease Co-Occurrences in Patents



► PubChem

9.5 Chemical-Gene Co-Occurrences in Patents



► PubChem

10 Classification



10.1 MeSH Tree



► Medical Subject Headings (MeSH)

10.2 UN GHS Classification



► GHS Classification (UNECE)

11 Information Sources



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ALL SOURCES



1. European Chemicals Agency (ECHA)

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<https://echa.europa.eu/web/guest/legal-notice>

8-benzyl-2-[(furan-2-yl)methyl]-6-phenyl-3H,7H-imidazo[1,2-a]pyrazin-3-one (EC: 846-449-3)

<https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/292195>

8-benzyl-2-[(furan-2-yl)methyl]-6-phenyl-3H,7H-imidazo[1,2-a]pyrazin-3-one

<https://echa.europa.eu/substance-information/-/substanceinfo/100.283.478>

2. Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J3.661.436F

3. Nature Chemical Biology

<https://pubchem.ncbi.nlm.nih.gov/substance/475777106>

4. PubChem

<https://pubchem.ncbi.nlm.nih.gov>

5. Medical Subject Headings (MeSH)

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

furimazine

<https://www.ncbi.nlm.nih.gov/mesh/2099610>

MeSH Tree

<http://www.nlm.nih.gov/mesh/meshhome.html>

Luminescent Agents

<https://www.ncbi.nlm.nih.gov/mesh/68049408>

6. GHS Classification (UNECE)

GHS Classification Tree

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

7. PATENTSCOPE (WIPO)

SID 497545261

<https://pubchem.ncbi.nlm.nih.gov/substance/497545261>