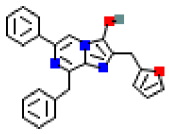
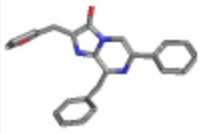
PubChem

COMPOUND SUMMARY

Furimazine

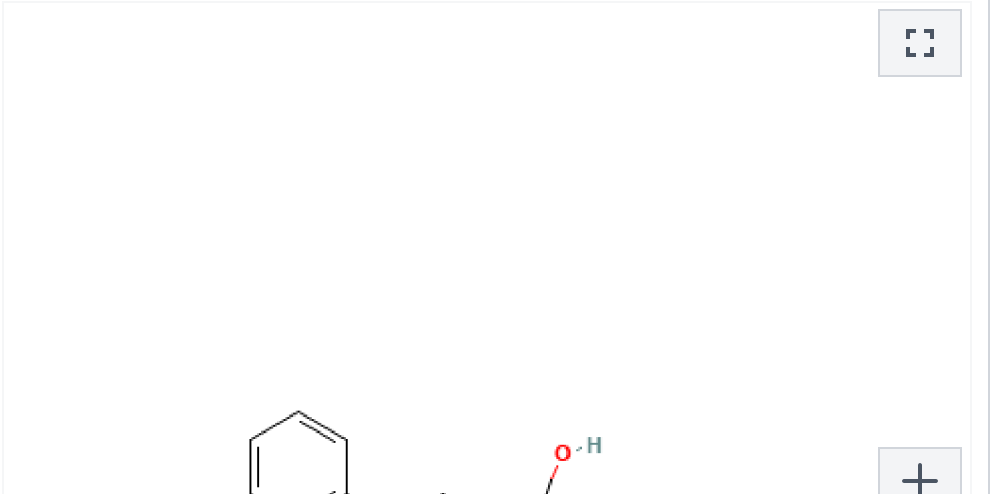
PubChem CID	136008305
Structure	 2D  3D
Chemical Safety	 Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_{24}H_{19}N_3O_2$
Synonyms	Furimazine 1374040-24-0 8-benzyl-2-(furan-2-ylmethyl)-6-phenylimidazo[1,2-a]pyrazin-3(7H)-one 8-Benzyl-2-[(furan-2-yl)methyl]-6-phenylimidazo[1,2-a]pyrazin-3(7H)-one 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: 2019-01-21 Modify: 2024-11-09

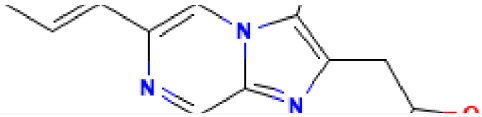
Contents

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

First Previous Conformer 1 of 10 Next Last

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

$C_{24}H_{19}N_3O_2$

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

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	63.6Å²	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)	 Irritant
Signal	Warning
GHS Hazard Statements	H302 (100%): Harmful if swallowed [Warning Acute toxicity, oral] H315 (100%): Causes skin irritation [Warning Skin corrosion/irritation] H319 (100%): Causes serious eye irritation [Warning Serious eye damage/eye irritation] H335 (100%): May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation]
Precautionary Statement Codes	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 (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)

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:

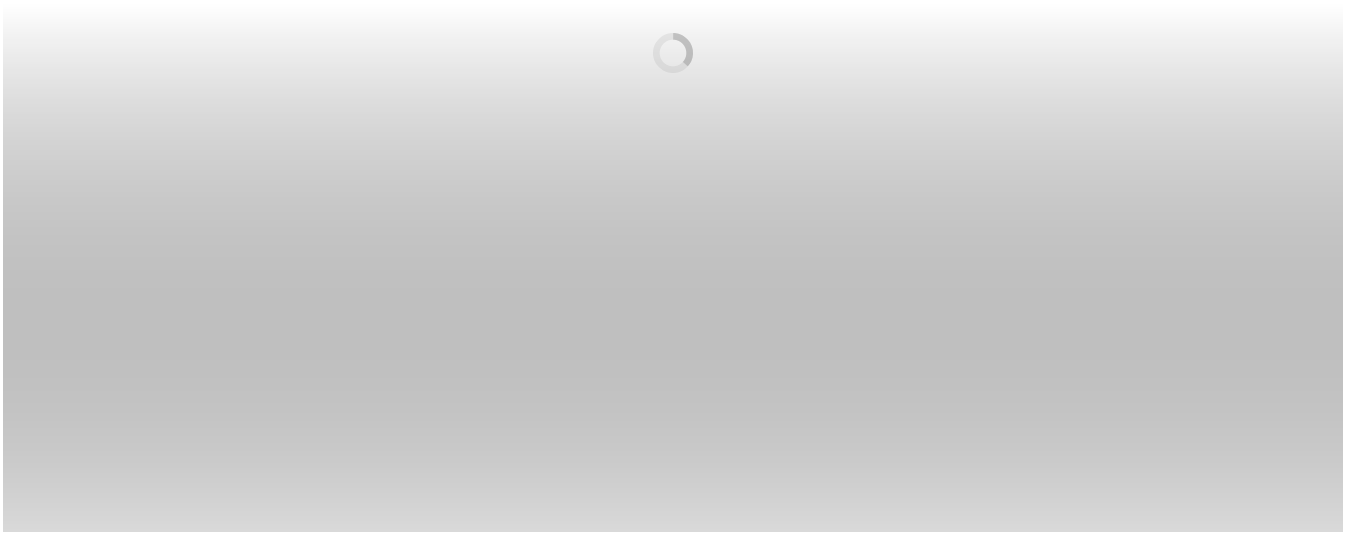
https://patentscope.wipo.int/search/en/result.jsf?inchikey=HTBLMRUZSCCOLL-UHFFFAOYSA-N

- 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

FILTER BY SOURCE

ALL SOURCES

1. European Chemicals Agency (ECHA)

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)

   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