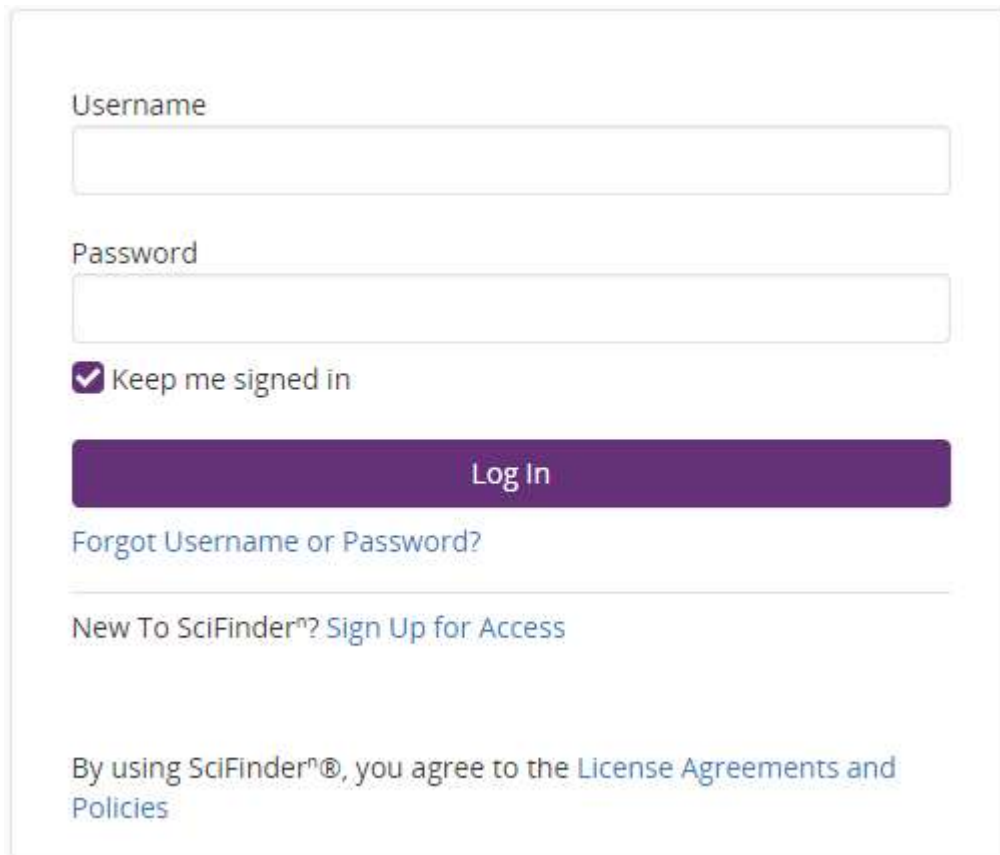


Congratulations on purchasing a license for SciFinderⁿ, the world's most trusted and comprehensive chemistry relevance engine in the industry. Here's how to get started:

Logging to SciFinderⁿ


- Go to [SciFinderⁿ homepage](https://scifinder-n.cas.org/) (https://scifinder-n.cas.org/)
- Login with your username and password
 - First-time commercial users are able to self-register. You can request additional resources for assistance.



The screenshot shows the SciFinder login interface. It features a 'Username' input field, a 'Password' input field, and a checked checkbox for 'Keep me signed in'. Below these is a prominent purple 'Log In' button. Underneath the button are links for 'Forgot Username or Password?' and 'New To SciFinderⁿ? Sign Up for Access'. At the bottom, there is a statement: 'By using SciFinderⁿ®, you agree to the [License Agreements and Policies](#)'.

Getting Started

- **Search:** SciFinderⁿ features a new streamlined search interface, including advanced text and structure search functionalities.



The diagram illustrates the search interface with three numbered steps:

1. Select the type of search that you want to perform. (Points to the search type dropdown menu with options: All, Substances, Reactions, References, Suppliers)
2. Enter text query. (Points to the 'Enter a query...' input field)
3. Execute search. (Points to the search button)

Additional features shown include a 'Draw' button for structure queries and an 'OR' separator between the text and structure query options. The search bar is labeled 'Search by Keyword, CAS RN, Patent Number, etc.'

- History:** SciFinderⁿ tracks your searches in a dynamic way, and allows you to quickly find your previous work. You can also easily save and set-up alerts for your searches.

- Reference:** Reference search makes use of the most advanced chemically intelligent algorithm in the world. The display features new visualizations, dynamic facets, and an easy-to-use layout
 - Full text acquisition options are available on the reference search page

Substances: Substance search returns results in an intuitive layout. The display highlights most relevant hits, critical property information, and high resolution images of structures.

- Clicking on substance details take you to the full detailed records available on SciFinderⁿ.

Retrieve data related to answers. Download answers to an external file. Change how answers are displayed.

Select type of structure match. Select filters to focus answers.

Go to Substance Detail screen. View Key Physical Properties on Substance Detail screen.

Share answers by emailing link. Save answers.

Retrieve data for substance.

View Full

Substances (6)

Structure Match

As Drawn (1)

Substructure (6)

Similarity (3,437)

Filter by

Commercial Availability

Available (1)

Not Available (5)

Reaction Role

Product (2)

Reactant (4)

Reference Role

Biological Study (1)

Preparation (2)

Prophetic in Patents (1)

Reactant or Reagent (4)

Uses (1)

Number of Components

Substance Class

Molecular Weight

1219937-98-0

View Detail

Key Physical Properties

Key Physical Properties	Value	Condition
Molecular Weight	404.4±30.0	Press: 760 Torr
Boiling Point (Predicted)	404.4±30.0 °C	
Density (Predicted)	1.504±0.06 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	13.86±0.70	Most Acidic Temp: 25 °C

C₁₁H₉ClFNO₂

Cyclopropanecarbonyl chloride, 1-[[[4-fluorophenyl]amino]carbonyl]-

29 References 98 Reactions 1 Supplier

1416321-38-4

View Detail

Key Physical Properties

Key Physical Properties	Value	Condition
Molecular Weight	276.09	-
Boiling Point (Predicted)	428.6±45.0 °C	Press: 760 Torr
Density (Predicted)	1.600±0.06 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	13.18±0.70	Most Acidic Temp: 25 °C

C₁₁H₈Cl₂FNO₂

Cyclopropanecarbonyl chloride, 1-[[[3-chloro-4-fluorophenyl]amino]carbonyl]-

1 Reference 2 Reactions 0 Suppliers

Reactions: Reaction Search displays relevant schema as well as key synthetic information.

- Clicking on the **Reaction Details** will allow you to see step-by-step instructions and more detail on the reaction.

Go to Reactions screen. View previous or next reaction.

Download answers to an external file. Share answers by emailing link. Save data.

Click any substance image or name to display substance menu. Use menu options to view substance details (CAS Registry Number), zoom image (magnifier), retrieve associated information (Reactions, Suppliers, References), or copy substance to editor (Edit Substance).

Retrieve suppliers for substance.

View reaction reference on Reference Detail screen.

View full-text PDF for the patent reference or Patent Family members.

Access other full-text options.

Return to All Reaction Schemes

Reaction Detail (Scheme 1, Reaction 2 of 20)

Suppliers (2) Suppliers (25) Suppliers (55)

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	Potassium carbonate	-	Tetrahydrofuran Water	10 min, > 30 °C
2	Water	-	-	10 h, 15 - 30 °C

CAS Reaction Number 31-365-CAS-4160897

Notes

alternative reaction conditions shown

Experimental Protocols

Experimental Procedure

Preparation of N-(4-((6,7-bis(methoxyloxy)quinolin-4-yl)oxy)phenyl)-N'-(4-fluorophenyl)cyclopropane-1,1-dicarboxamide

The solution from the previous step containing 1-(4-fluoro-phenyl)carbamoyl-cyclopropanecarbonyl chloride was added to a mixture of 4-(6,7-dimethoxy-quinoline-4-yl)oxyphenylamine (3.0 kg), and potassium carbonate (4.0 kg) in THF (27.0 kg), and water (13.0 kg) at a rate such that the hatch temperature did not exceed 3.0 °C. When the reaction was complete (approximately 10 minutes), water (74.0 kg) was added. The mixture was stirred at 15 to 300 °C for approximately 10 hours, which resulted in the precipitation of the product. The product was recovered by filtration, washed with a pre made solution of THF (11.0 kg) and water (24.0 kg), and dried at approximately 65 °C under vacuum for approximately 12 hours to afford the title compound. Yield (free base, 5.0 kg). ¹H NMR (400 MHz, d₆-DMSO): δ 10.2 (s, 1 H), 10.05 (s, 1H), 8.4 (s, 1H), 7.8 (m, 2H), 7.65 (m, 2H), 7.5 (s, 1H), 7.35 (s, 1H), 7.25 (m, 2H), 7.15 (m, 2H), 6.4 (s, 1H), 4.0 (d, 6H), 1.5 (s, 4H) LC/MS: M+H = 502.

Reference

Method of treating cancer and bone cancer pain

View Reference Detail

By: Schwab, Gisela; et al

World Intellectual Property Organization, WO2012151326 A1 2012-11-08

PATENTPAK Full Text

Patent Information

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