

# Chemical Inventory

Chemaxon UGM May 2012

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CHEMICAL  
INVENTORY

# Agenda

- Presentation
- Jchem integration
- Core functionality
- Benefits
- Further information



# Presentation

- [Chemicalinventory.org](https://chemicalinventory.org)
- Product state: Commercial product
- Target audience
  - Industry and universities



# Jchem integration

- Integration example:
  - Search
  - Search result
  - Compound details



# Jchem integration

**Search**

Search Term

Formula

Cas

Mol Weight

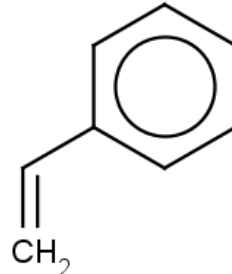
Density

Registered Date

Registered By

Search Method

File Edit View Insert Atom Bond Structure Tools Help



CH<sub>2</sub>

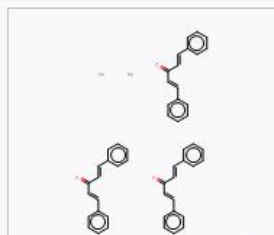
Search >> Cancel

The image shows a software interface for searching chemical structures. On the left, there is a search panel with fields for Search Term (pallad), Formula, Cas, Mol Weight, Density, Registered Date, Registered By, and Search Method (SUBSTRUCTURE). The main window displays a chemical structure of styrene (vinylbenzene) with a benzene ring and a vinyl group (-CH=CH<sub>2</sub>). The interface includes a menu bar (File, Edit, View, Insert, Atom, Bond, Structure, Tools, Help) and a toolbar with various icons for editing and viewing. A vertical toolbar on the right contains buttons for elements H, C, N, O, S, F, P, Cl, Br, I. At the bottom, there are buttons for 'Search >>' and 'Cancel'.



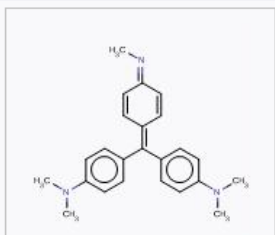
# Jchem integration

## Compound List



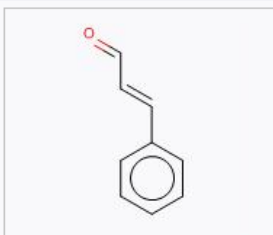
**TRIS(DIBENZYLIDENE)ACETONE OR Pd2DBA3**

CAS:  
Formula:  $C_{51}H_{42}O_3Pd_2$   
Mw: 915.72



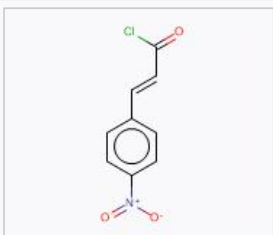
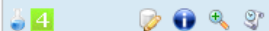
**METHYL VIOLET**

CAS:  
Formula:  $C_{24}H_{27}N_3$   
Mw: 357.4913



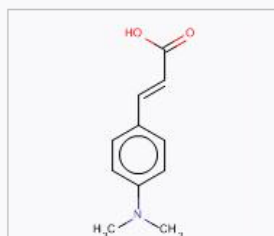
**TRANS-CINNAMALDEHYDE**

CAS: 14371-10-9  
Formula:  $C_9H_8O$   
Mw: 132.1592



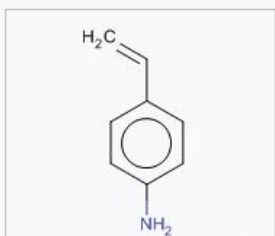
**TRANS-4-NITROCINNAMOYL CHLORIDE**

CAS: 61921-33-3  
Formula:  $C_9H_6ClNO_3$   
Mw: 211.602



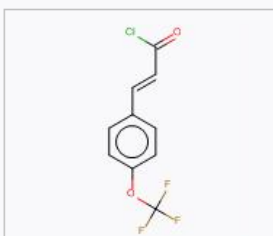
**4-(DIMETHYLAMINO)CINNAMIC ACID**

CAS: 1552-96-1  
Formula:  $C_{11}H_{13}NO_2$   
Mw: 191.2264



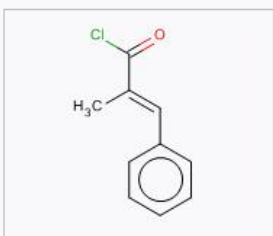
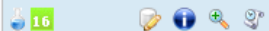
**4-VINYLANILINE**

CAS: 1520-21-4  
Formula:  $C_8H_9N$   
Mw: 119.1638



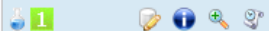
**3-[4-(TRIFLUOROMETHOXY)PHENYL]ACRYLOYL CHLORIDE**

CAS: 306936-02-7  
Formula:  $C_{10}H_6ClF_3O_2$   
Mw: 250.602



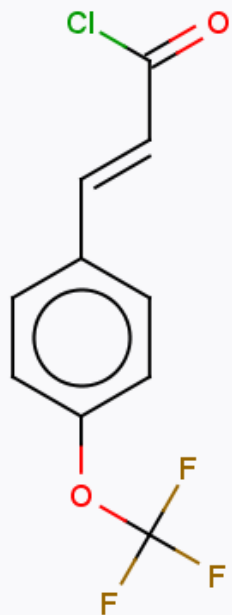
**(E)-2-METHYL-3-PHENYLPROP-2-ENOYL CHLORIDE**

CAS: 35086-87-4  
Formula:  $C_{10}H_9ClO$   
Mw: 180.631



# Jchem integration

## 3-[4-(TRIFLUOROMETHOXY)PHENYL]PROP-2-ENOYL CHLORIDE



Compound Name	3-[4-(TRIFLUOROMETHOXY)PHENYL]PROP-2-ENOYL CHLORIDE
Formula	C <sub>10</sub> H <sub>6</sub> ClF <sub>3</sub> O <sub>2</sub>
Cas	306936-02-7
Mol Weight	250.602
Density	0g/cm <sup>3</sup>
Registered Date	04/08/2010 16:41:10
Registered By	
Remark	

## Container List (3-[4-(TRIFLUOROMETHOXY)PHENYL]PROP-2-ENOYL CHLORIDE)

Id	Owner	Home	Location	Remark	Quantity	
11462	duke /	Chemical Storage Room     root 0     Root PO1	Home		13.54 g	<input type="button" value="Check Out"/> 



# Jchem integration

- Further integration:
  - Direct compound download
    - Use CAS or name to search and import and update compound information.





# Core functionality

- Full inventory tracking
- Structure drawing and search
- Track compounds and containers
- Powerful search facility
- Automated compound registration system features
- Dynamic label print
- Report generation of essential data
- Audit trail and history on all data
- Use barcodes for labels
- External links - MSDS
- Advanced administration module
- Automated reorder process
- Quick access



# Benefits

- **Workflow**
  - Enhance workflow and minimize time wasted searching for chemicals.
- **Financial**
  - Ensure that chemicals in stock is used before reordering.
- **Environmental**
  - Avoid unnecessary environmental impact by having an optimized inventory.



## Furhter information

- <http://www.chemicalinventory.org>
  - Online demo
- Email: [info@chemicalinventory.org](mailto:info@chemicalinventory.org)
- +45 8161 6108

