Chemical Inventory

Chemaxon UGM May 2012
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Agenda

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

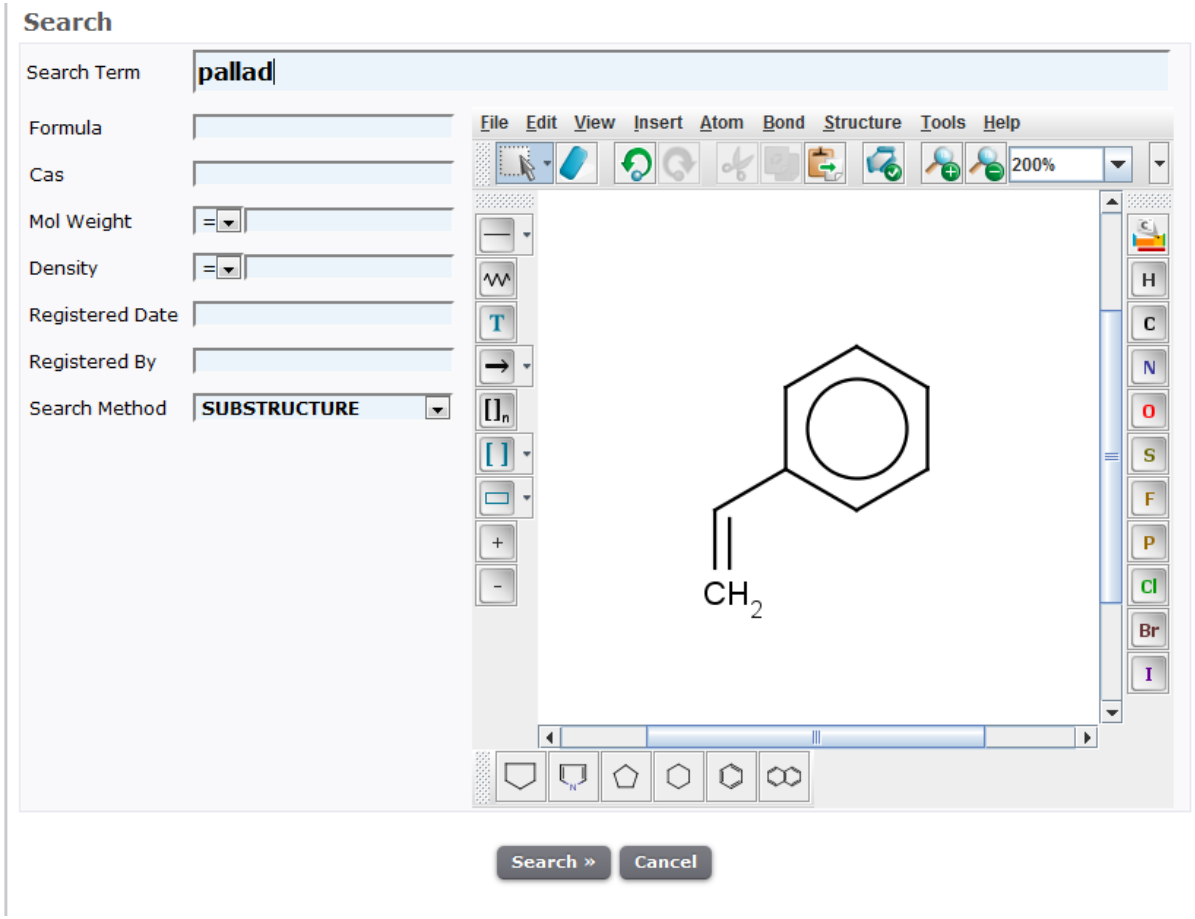
Presentation

- Chemicalinventory.org
- Product state: Commercial product
- Target audience
  - Industry and universities

Jchem integration

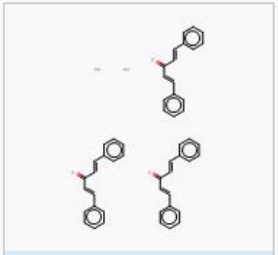
- Integration example:
  - Search
  - Search result
  - Compound details

Jchem integration



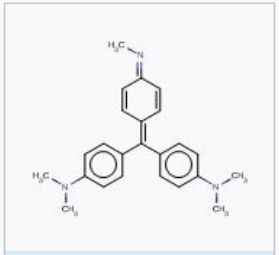
Jchem integration

Compound List



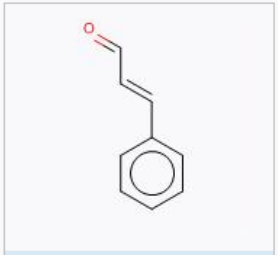
TRIS(DIBENZYLIDINEA(OR PD2DBA3

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



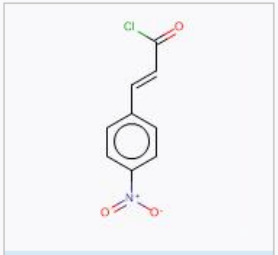
METHYL VIOLET

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



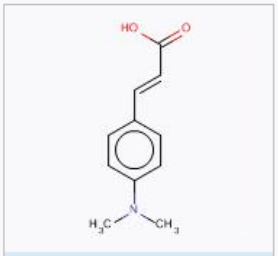
TRANS-CINNAMALDEHYDE

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



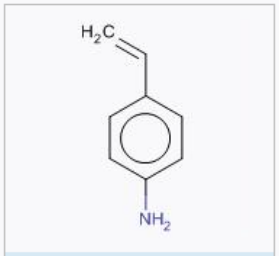
TRANS-4-NITROCINNAMOYL CHLORIDE

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



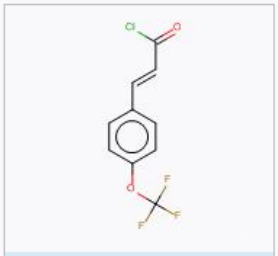
4-(DIMETHYLAMINO)CI ACID

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



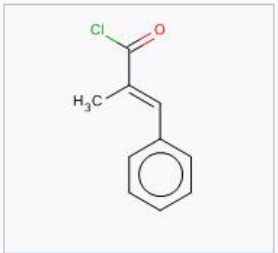
. 4-VINYLANILINE

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



3-[4-(TRIFLUOROMETH 2-ENOYL CHLORIDE

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

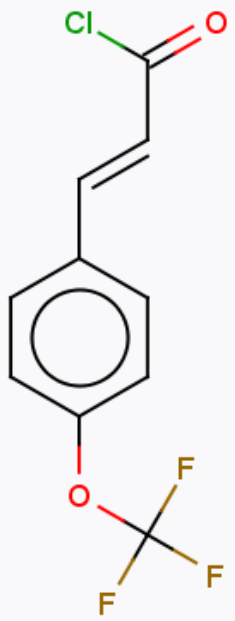


(E)-2-METHYL-3-PHENYLPROP-2-ENOYL CHLORIDE

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	**$C_{10}H_6ClF_3O_2$**
Cas	**306936-02-7**
Mol Weight	**250.602**
Density	**0g/cm3**
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	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
- +45 8161 6108