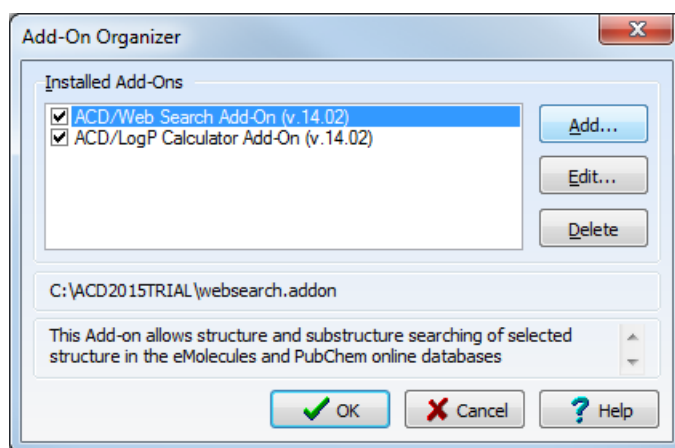


EPA's Interactive Chemical Safety for Sustainability (iCSS) Database

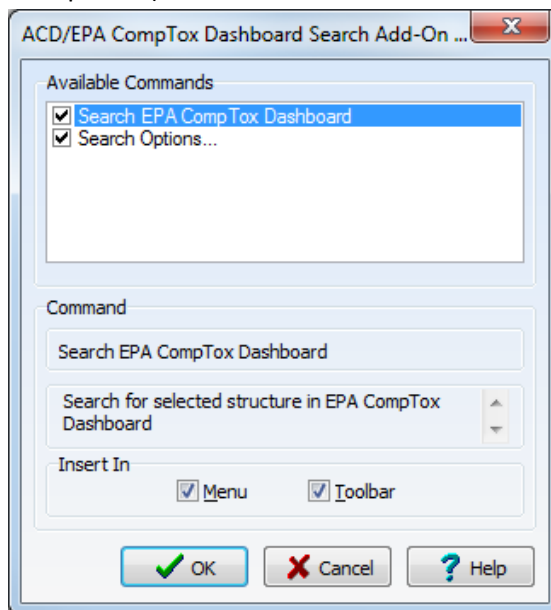
Add-on for ACD/ChemSketch
 Advanced Chemistry Development, Inc.
 Toronto, ON, Canada
www.acdlabs.com

Installation Instructions

1. Download the EPA iCSS add-on file from www.acdlabs.com/resources/freeware. Ensure you have unzipped and located the file on your hard drive.
2. Open ACD/ChemSketch
3. From the **Options** menu, choose **Add-on Organizer**. In the **Add-on Organizer** dialog box that appears, click **Add**, and browse to the location of the *epa.addon* file.



4. Choose your installation options (we recommend the default settings) and click **OK**.



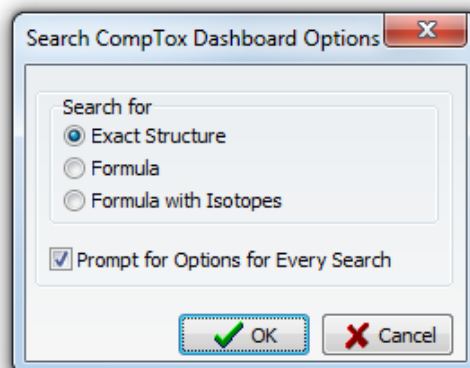
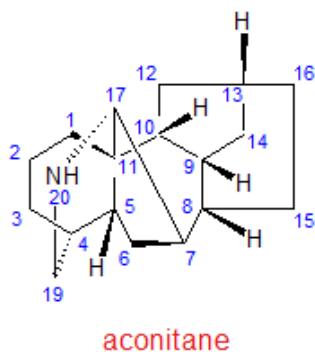
5. The *EPA CompTox Dashboard Search Add-on* should now be listed in your Add-on Organizer. Click **OK**.

Using the EPA Add-on

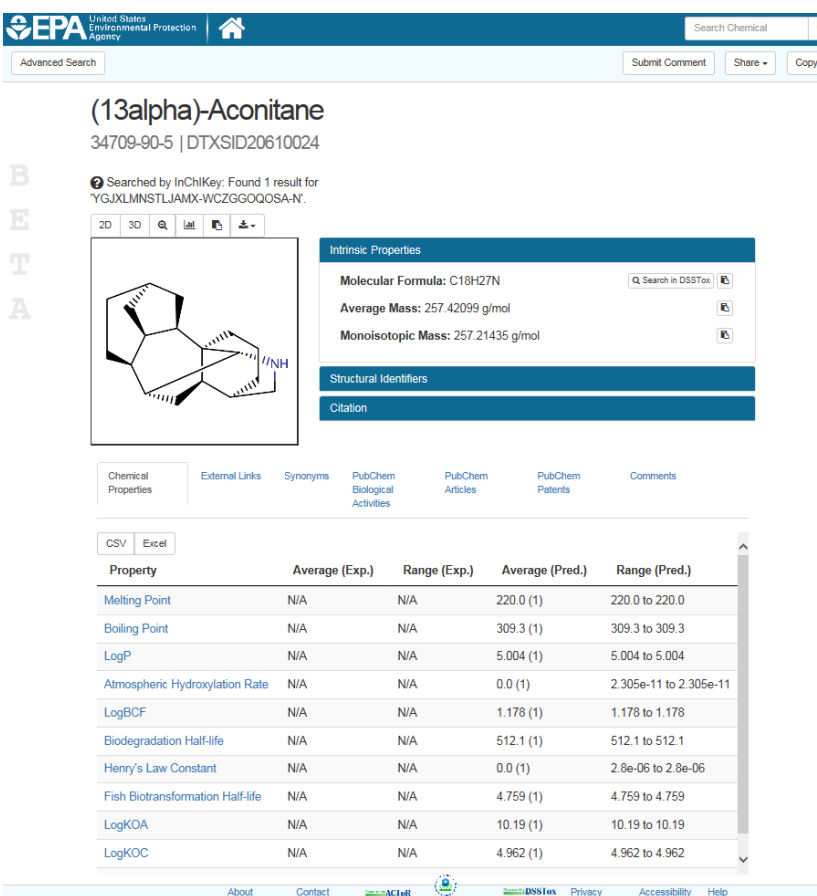
1. With a structure drawn in ChemSketch, from the Add-on toolbar, click **EPA**.



2. Choose the search options and click **OK**.



3. The database search results appear in your browser window.



(13 α)-Aconitane
34709-90-5 | DTXSID20610024

Search by InChIKey: Found 1 result for YGJXLMNSTLJAMX-WCZGGQOSA-N.

Intrinsic Properties

Molecular Formula:	C ₁₈ H ₂₇ N
Average Mass:	257.42099 g/mol
Monoisotopic Mass:	257.21435 g/mol

Structural Identifiers

Citation

Chemical Properties | External Links | Synonyms | PubChem Biological Activities | PubChem Articles | PubChem Patents | Comments

Property	Average (Exp.)	Range (Exp.)	Average (Pred.)	Range (Pred.)
Melting Point	N/A	N/A	220.0 (1)	220.0 to 220.0
Boiling Point	N/A	N/A	309.3 (1)	309.3 to 309.3
LogP	N/A	N/A	5.004 (1)	5.004 to 5.004
Atmospheric Hydroxylation Rate	N/A	N/A	0.0 (1)	2.305e-11 to 2.305e-11
LogBCF	N/A	N/A	1.178 (1)	1.178 to 1.178
Biodegradation Half-life	N/A	N/A	512.1 (1)	512.1 to 512.1
Henry's Law Constant	N/A	N/A	0.0 (1)	2.8e-06 to 2.8e-06
Fish Biotransformation Half-life	N/A	N/A	4.759 (1)	4.759 to 4.759
LogKOA	N/A	N/A	10.19 (1)	10.19 to 10.19
LogKOC	N/A	N/A	4.962 (1)	4.962 to 4.962