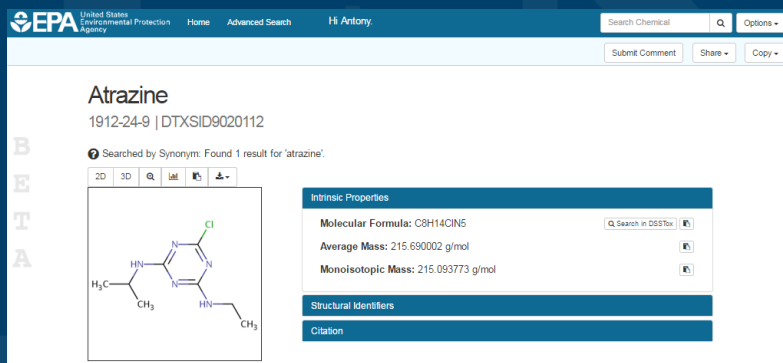


An Introduction to the iCSS Chemistry Dashboard



The screenshot shows the EPA iCSS Chemistry Dashboard for Atrazine. The page header includes the EPA logo, navigation links (Home, Advanced Search), and the user name 'Hi Antony'. A search bar contains 'Atrazine' and there are buttons for 'Submit Comment', 'Share', and 'Copy'. The main content area displays 'Atrazine' with its CAS number '1912-24-9' and DTSID 'DTXSID9020112'. Below this, it states 'Searched by Synonym: Found 1 result for 'atrazine''. There are icons for 2D, 3D, and other views. A chemical structure of Atrazine is shown, featuring a central 1,3,5-triazine ring with a chlorine atom at position 4, an isopropylamino group at position 6, and an ethylamino group at position 2. To the right of the structure is a table of 'Intrinsic Properties':

Intrinsic Properties	
Molecular Formula:	C ₈ H ₁₄ ClN ₅
Average Mass:	215.690002 g/mol
Monoisotopic Mass:	215.093773 g/mol

Below the table are sections for 'Structural Identifiers' and 'Citation'.

May 26, 2016

Antony Williams and Kamel Mansouri
National Center for Computational Toxicology

The iCSS Chemistry Dashboard

PRIMARY GOALS

- Deliver a web-based application serving up the chemistry related data used by our team
- Provide public access to the results of over a decade of curation work reviewing environmental chemistry data
- Provide access to the results of our QSAR modeling work
- Deliver a central hub to link together websites of interest
- All data to be available as Open Data for download/reuse

SECONDARY GOAL

- To develop a cheminformatics architecture to serve as a high quality chemical foundation for all NCCT tools and data

iCSS Chemistry Dashboard

<https://comptox.epa.gov>



B
E
T
A

Chemistry Dashboard

Search a chemical by systematic name, synonym, CAS number, or InChIKey



Single component search Ignore isotopes

Need more? Use [advanced search](#).

720 Thousand Chemicals



DSSTox Chemistry Content



Mutation Research/Fundamental and
Molecular Mechanisms of Mutagenesis

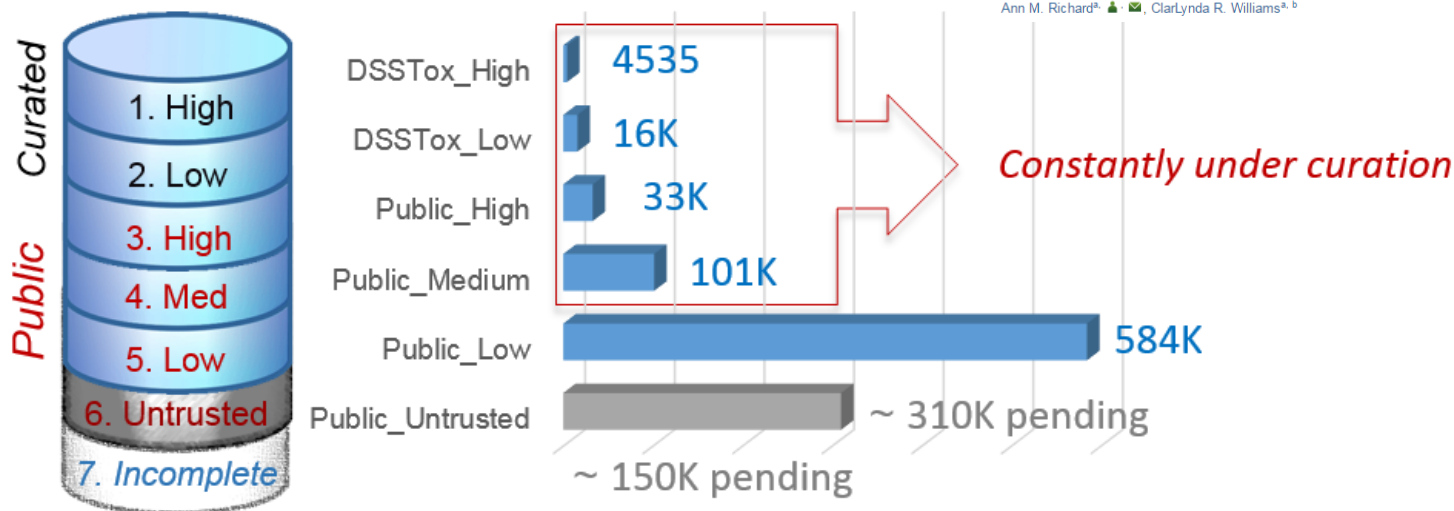
Volume 499, Issue 1, 29 January 2002, Pages 27-52



Mutation Research Frontiers

Distributed structure-searchable toxicity (DSSTox) public
database network: a proposal

Ann M. Richard^a, ClarLynda R. Williams^{a, b}



QC Levels

DSSTox_High:	Hand curated and validated
DSSTox_Low:	Hand curated and confirmed using multiple public sources
Public_High:	Extracted from EPA SRS and confirmed to have no conflicts in ChemID and PubChem
Public_Medium:	Extracted from ChemID and confirmed to have no conflicts in PubChem
Public_Low:	Extracted from ACToR or PubChem
Public_Untrusted:	Postulated, but found to have conflicts in public sources

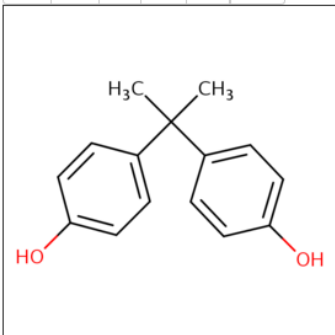
iCSS Chemistry Dashboard

Bisphenol A

80-05-7 | DTXSID7020182

Searched by Synonym: Found 1 result for 'bisphenol A'.

2D 3D    



Intrinsic Properties

Molecular Formula: C₁₅H₁₆O₂



Average Mass: 228.291 g/mol



Monoisotopic Mass: 228.11503 g/mol



Structural Identifiers

Citation

Chemical Properties

External Links

Synonyms

PubChem Biological Activities

PubChem Articles

PubChem Patents

Comments

CSV

Excel

Property	Average (Exp.)	Range (Exp.)	Average (Pred.)	Range (Pred.)
Solubility	0.001 (1)	0.0005257 to 0.0005257	0.38 (2)	0.003875 to 0.7565
Melting Point	154.929 (7)	153.0 to 158.0	144.033 (3)	131.8 to 158.0
Boiling Point	200.0 (1)	200.0 to 200.0	348.95 (2)	334.4 to 363.5
LogP	3.357 (3)	3.32 to 3.431	3.524 (3)	3.205 to 3.727
Atmospheric Hydroxylation Rate	N/A	N/A	0.0 (1)	4.237e-11 to 4.237e-11
LogBCF	1.64 (1)	1.64 to 1.64	1.376 (1)	1.376 to 1.376
Biodegradation Half-life	N/A	N/A	15.11 (1)	15.11 to 15.11
Henry's Law Constant	N/A	N/A	0.0 (1)	6.972e-07 to 6.972e-07

About

Contact

 ACToR



 DSSTox

Privacy

Accessibility

Help

>500,000 chemical names

- Names, numeric identifiers and synonyms critical for:
 - Searching database
 - Integrating to external searches
 - Supporting text-mining approaches

[Chemical Properties](#) [External Links](#) [Synonyms](#) [PubChem Biological Activities](#) [PubChem Articles](#) [PubChem Patents](#) [Comments](#)

Found 75 synonyms

Legend: **Valid Synonyms** *Good Synonyms* *Other Synonyms* [Copy all Synonyms](#)

Bisphenol A

4,4'-(Propane-2,2-diyl)diphenol
phenol, 4,4'-(1-methylethylidene)bis-

BPA

4,4'-Propane-2,2-diylidiphenol
Phenol, 4,4'-(1-methylethylidene)bis-

80-05-7 [CAS-RN](#)

4-06-00-06717 [Beilstein Registry Number](#)

[About](#)

[Contact](#)



Powered by ACToR



Powered by DSSTox

[Privacy](#)

The iCSS Chemistry Dashboard
















 United States Environmental Protection Agency 



Bisphenol A

80-05-7 | DTXSID7020182

B
E
T
A

[Chemical Properties](#) **[External Links](#)** [Synonyms](#) [PubChem Biological Activities](#) [PubChem Articles](#)

General	Toxicology	Publications	Prediction
 EPA Substance Registry Service	 ToxCast Dashboard 2	 Google Scholar	 Chemicalize
 PubChem	 CTD	 Google Patents	
 ChemSpider	 EDSP Dashboard	 PubMed	
 CPCat	 Gene-Tox		
 DrugBank			
 National Environmental Methods Index			
 ChemView			

About Contact   Privacy Accessibility Help

Make maintenance easy... Please suggest new ones!

Edit Link

Name

National Environmental Methods Index

Url

http://www.nemi.gov/methods/keyword/?keyword_search_field=%s

Parameter

CAS

Category

General

Select icon

Search Icon


Description

NEMI is a searchable database that allows scientists and managers to find and compare analytical and field methods for all phases of environmental monitoring.

Back

Update External link

Use this database to get information on chemical health and safety data received by EPA and EPA's assessments and regulatory actions for specific chemicals under the Toxic Substances Control Act (TSCA).

 ChemView

ChemView

Information and data sources made available via ChemView are currently undergoing system upgrades or maintenance. During this time, some pages of the site (searchable databases, pdfs, etc.) may not be available. We apologize for the inconvenience and thank you for your patience and understanding.

Use this database to get information on chemical health and safety data received by EPA and EPA's assessments and regulatory actions for specific chemicals under the Toxic Substances Control Act (TSCA). ChemView contains no confidential business information (CBI).

If you do not receive results for a particular chemical, it does not mean EPA does not have information on that chemical; the data may not be posted yet but will be available in the future as EPA continues to populate the database.

- Learn more and find additional information about EPA's efforts in assessing and managing chemicals
- Read the ChemView User's Guide and Web Service Information
- To continuously improve ChemView, Contact Us with your feedback.

Data last updated on 3/24/2016

CHEMICALS **ENFORCEMENT** DASHBOARD OTHER SOURCES

Select Search Criteria:
Select Chemical Search Criteria and desired Output Selections.

Generate Results | Export Results | Clear All Entries

Chemical Information | Clear Chemical Information


starts with | exact | contains

Chemical name or Chemical Identifier

1

Show 10 entries

Search:

Structure	Chemical Name/ Chemical Identifier	Data Submitted to EPA	EPA Actions	Manufacturing, Processing, Use or Release
	▼ Bisphenol A 80-05-7	■ ■ ■	View for All	■ ■ ■

Showing 1 to 1 of 1 entries

First Previous 1 Next Last

E-mail Url Print Help Export

The iCSS Chemistry Dashboard

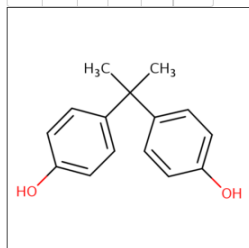


Bisphenol A

80-05-7 | DTXSID7020182

Searched by Synonym: Found 1 result for 'bisphenol A'.

2D 3D



Intrinsic Properties

Molecular Formula: C₁₅H₁₆O₂

Average Mass: 228.291 g/mol



Monoisotopic Mass: 228.11503 g/mol

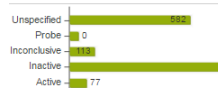


Structural Identifiers

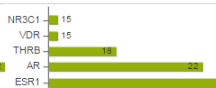
Citation

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

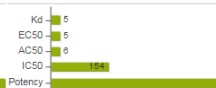
BioActivity Outcomes



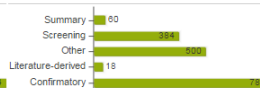
Top Targets



BioActivity Types



BioAssay Types



Structure	Substance SID	Activity			Compound Name	Bioassay Name
		Outcome	Type	Value [µM]		
	14214949	Inconclus.	Potency	96.099	Bisphenol A	qHTS assay to identify small molecule antagonists of the retinoic acid receptor (RAR) signaling pathway: Summary [AID:115955; Type: Summary]
	14214949	Active	Potency	34.974	Bisphenol A	qHTS assay to identify small molecule antagonists of the retinoid-related orphan receptor gamma (ROR-gamma) signaling pathway [AID:115953; Type: Confirmatory]
	14214949	Inactive	Potency		Bisphenol A	qHTS assay to identify small molecule antagonists of the retinoid-related orphan receptor gamma (ROR-gamma) signaling pathway - cell viability counter screen [AID:115952; Type: Confirmatory]
	14214949	Inactive	Potency		Bisphenol A	qHTS assay to identify small molecule agonists of the endoplasmic reticulum stress response signaling pathway: Summary [AID:115949; Type: Summary]

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Expt'l and Predicted PhysChem Data

Chemical Properties: LogP
✕

	Average	Range
Experimental	2.617 (3)	2.61 to 2.632
Predicted	2.721 (3)	2.67 to 2.82

CSV
Excel

Property	Raw Result	Mean Result	Minimum Result	Maximum Result	Result Unit	Result Type	Source
Estimated Log Kow	2.82	2.82	2.82	2.82		predicted	EPI SUITE
LogP	2.632	2.632	2.632	2.632		experimental	Vitas-M
LogP	2.674	2.674	2.674	2.674		predicted	ACD/Labs
Measured Log Kow	2.61	2.61	2.61	2.61		experimental	EPI SUITE
Octanol-water partition coefficient	2.61	2.61	2.61	2.61		experimental	CURATED_PHYSP
Octanol-water partition	2.6699	2.67	2.67	2.67		predicted	NCCT_Models

Property	Average (Pred.)	Range (Pred.)
Estimated Log Kow	0.525 (2)	0.05716 to 0.9926
LogP	150.55 (2)	113.9 to 187.2
LogP	326.0 (2)	313.0 to 339.0
LogP	2.721 (3)	2.67 to 2.82
Measured Log Kow	0.0 (1)	1.711e-11 to 1.711e-11
Measured Log Kow	0.936 (1)	0.936 to 0.936
Measured Log Kow	4.921 (1)	4.921 to 4.921

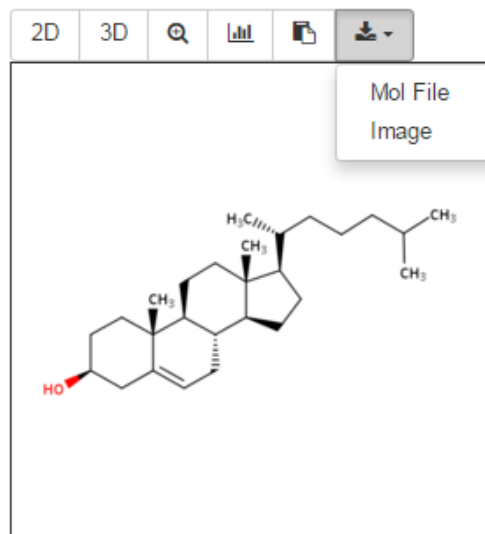
The PHYSPROP data sets are the publicly available data files underpinning the EPI Suite™ prediction models (<http://www.epa.gov/tsca-screening-tools/epi-suite™-estimation-program-interface>). The data were curated using a combination of manual and automated processing routines with only the highest quality data reported in this database. These data were utilized, in combination with other datasets where available, in the development of the NCCT Models provided via this ICSS Chemistry Dashboard. This partition coefficient is a ratio of concentrations of unionized compound between the two liquid phases. This property is the Octanol-Water partition coefficient, log Kow.

Data sharing and access

Cholesterol

57-88-5 | DTXSID3022401

Searched by Synonym: Found 1 result for 'cholesterol'.



Chemical Properties: LogP


	Average	Range
Experimental	3.357 (3)	3.32 to 3.431
Predicted	3.524 (3)	3.205 to 3.727

CSV Excel

Property	Raw Result	Mean Result	Minimum Result	Maximum Result	Result Unit	Result Type	Source
Estimated Log Kow	3.64	3.64	3.64	3.64		predicted	EPI SUITE
LogP	3.431	3.431	3.431	3.431		experimental	Vitas-M
LogP	3.727	3.727	3.727	3.727		predicted	ACD/Labs
Measured Log Kow	3.32	3.32	3.32	3.32		experimental	EPI SUITE
Octanol-water partition coefficient	3.32	3.32	3.32	3.32		experimental	CURATED_PHYSP

Found 75 synonyms

Legend: **Valid Synonyms** *Good Synonyms* Other Synonyms

 Copy all Synonyms

Bisphenol A

4,4'-(Propane-2,2-diyl)diphenol

phenol, 4,4'-(1-methylethylidene)bis-

BPA

4,4'-Propane-2,2-diylidiphenol

Phenol, 4,4'-(1-methylethylidene)bis-

80-05-7 [CAS-RN](#)

4-06-00-06717 [Beilstein Registry Number](#)

UNII-MLT3645I99 [FDA Registry Number](#)

(4,4'-Dihydroxydiphenyl)dimethylmethane

New “NCCT Prediction Models”

- PhysChem properties to include in exposure modeling, augmenting with Toxcast data etc.
- Our approach to modeling:
 - Obtain high quality training sets
 - Apply machine learning approaches
 - Validate performance
 - Predict across full datasets

NCCT Model Development

- Dashboard access to cleaned data, the predicted data for all chemicals and ultimately real time models
- QSAR prediction models (kNN) produced for all properties
- >700k chemical structures pushed through NCCT_Models

Available Properties

- Solubility
- Melting Point
- Boiling Point
- LogP (KOWWIN: Octanol-water partition coefficient)
- Atmospheric Hydroxylation Rate
- LogBCF (Bioconcentration Factor)
- Biodegradation Half-life
- Henry's Law Constant
- Fish Biotransformation Half-life
- LogKOA (Octanol/Air Partition Coefficient)
- LogKOC (Soil Adsorption Coefficient)
- Vapor Pressure

Some statistics

- 15,809 chemicals in the LogP dataset
- CAS Checksum: 12163 valid, 3646 invalid (>23%)
- Valence errors: 322 Molfile vs 3782 SMILES (>24%)
- SMILES vs. Molfiles (structure check)
 - 133 SMILES cannot be converted (~1%)
 - 1279 differ in stereochemistry (~8%)
 - 362 “Covalent Halogens”
 - 191 differ as “tautomers”
 - 436 are different compounds (~3%)
- **Original Training Set: >2400; Curated Training Set > 14000**

Adding MORE Data

- Collect “Open Data” for various endpoints from:
 - *PubChem*
 - *Open Data Sources*
- Data already harvested and awaiting processing
- New models to be produced from expanded data sets

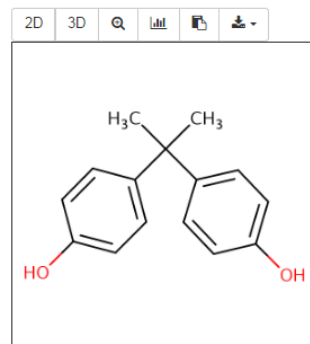
Connecting into the Dashboard

- Linkages into the Dashboard are simple: using the associated identifiers

Bisphenol A

80-05-7 DTXSID7020182

 Searched by Synonym: Found 1 result for 'bisphenol A'.



Intrinsic Properties

Structural Identifiers

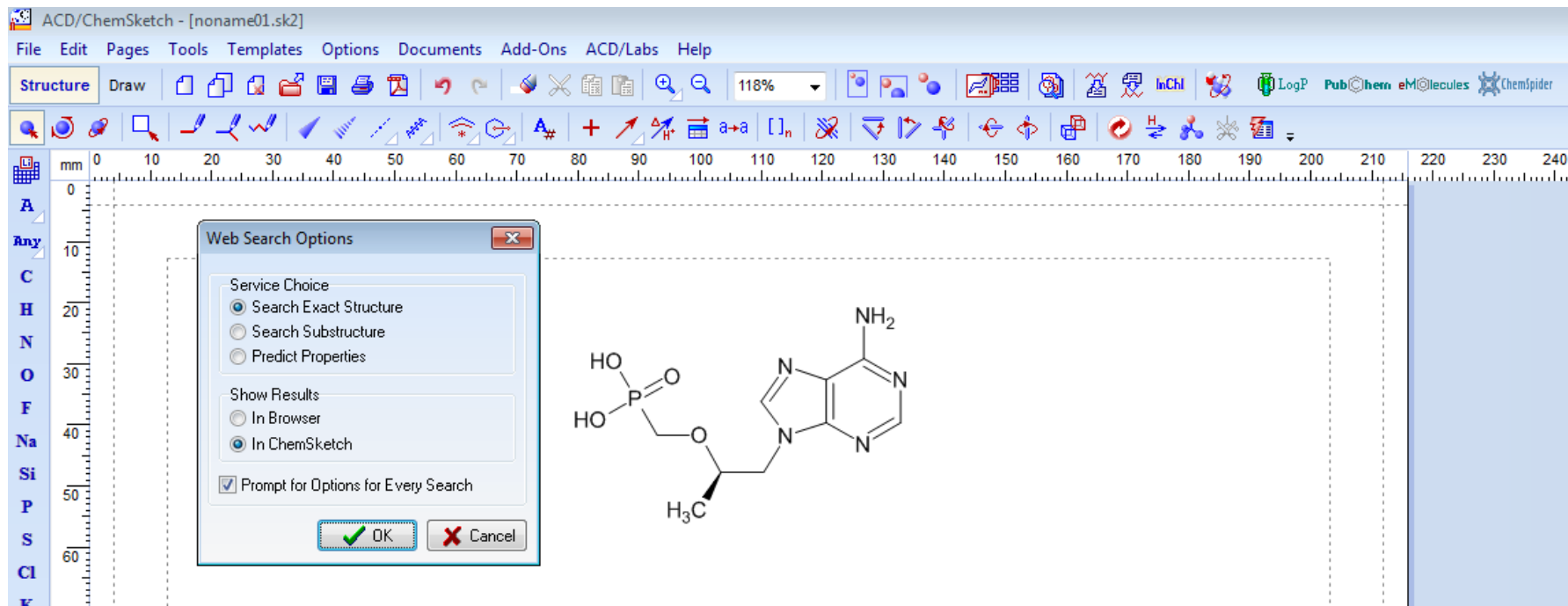
Citation

U.S. Environmental Protection Agency. iCSS Chemistry Dashboard.
<https://comptox.epa.gov/dashboard/DTXSID7020182> (accessed May 03, 2016),
Bisphenol A



- For integration we can supply files of structures/identifiers mapped to DTXSIDs. Contact us...
- PubChem, EBI's UNICHEM, ChemSpider and...

Desktop integration coming



The screenshot displays the ACD/ChemSketch software interface. The title bar reads "ACD/ChemSketch - [noname01.sk2]". The menu bar includes "File", "Edit", "Pages", "Tools", "Templates", "Options", "Documents", "Add-Ons", "ACD/Labs", and "Help". The toolbar contains various icons for drawing and editing, with a zoom level of 118%. The main workspace shows a chemical structure of a phosphonate derivative: C[C@@H](COP(=O)(O)O)CN1C=NC2=C(N)N=CN=C12. A "Web Search Options" dialog box is open, featuring the following settings:

- Service Choice:**
 - Search Exact Structure
 - Search Substructure
 - Predict Properties
- Show Results:**
 - In Browser
 - In ChemSketch
- Prompt for Options for Every Search

Buttons for "OK" and "Cancel" are visible at the bottom of the dialog box.

Next Release in June..

- June release delivery update
 - Faster searching
 - Improved navigation
 - New data types – integration to other NCCT apps
 - *In vitro* DB
 - Chemical and Product categories (CPCat)
 - Exposure Data
 - Expanded list of External Links
 - Calculation details for models

Type Ahead Search

Search input: ethylhexyl

- Ethylhexyl nitrate
- Ethylhexyl benzoate
- Ethylhexyl acid phosphate
- Ethylhexyl ester, 2,4-D, 2-
- Ethylhexyl methoxycinnamate
- Ethylhexyl p-methoxycinnamate
- Ethylhexyl benzyldioxopiperazyl acetate
- Ethylhexyl acrylate, vinylidene chloride copolymer
- Ethylhexyl acrylate, vinyl acetate, dioctyl maleate, acrylic acid polymer
- Ethylhexyl acrylate, methyl methacrylate, hydroxypropyl methacrylate, acrylic acid, acrylonitrile polymer

Search input: ethylhexyl p

- ethylhexyl palmitate
- ETHYLHEXYL PHTHALATE
- Ethylhexyl p-methoxycinnamate

New Table Displays

Chemical
Properties

External Links

Synonyms

Consumer
Usage

ToxCast in Vitro
Data

Exposure

Analytical

PubChem

Summary

CSV Excel

Solubility

Melting Point

Boiling Point

LogP

Atmospheric
Hydroxylation
Rate

LogBCF

Biodegradation
Half-life

Henry's Law
Constant

Fish
Biotransformati
on Half-life

LogKOA

LogKOC

Vapor
Pressure

Property	Average (Exp.)	Median (Exp.)	Range (Exp.)	Average (Pred.)	Median (Pred.)	Range (Pred.)	Result Unit
Solubility	0.026 (1)	0.0255	0.0255	14.8 (2)	14.8	0.146 to 29.4	mol/L
Melting Point	136 (13)	137	122 to 142	109 (2)	109	93.1 to 125	°C
Boiling Point	140 (2)	140	140	297 (2)	297	278 to 316	°C
LogP	1.19 (2)	1.19	1.19	1.33 (3)	1.41	1.13 to 1.44	-
Atmospheric Hydroxylation Rate	-	0	-	0 (1)	3.396e-11	3.396e-11	cm ³ /molecule-sec
LogBCF	-	0	-	0.619 (1)	0.619	0.619	-
Biodegradation Half-life	-	0	-	3.54 (1)	3.54	3.54	days
Henry's Law Constant	-	0	-	0 (1)	3.095e-05	3.095e-05	atm-m ³ /mole
Fish Biotransformation Half-life	-	0	-	0.114 (1)	0.114	0.114	days

New Table Displays

- Chemical Properties
- External Links
- Synonyms
- Consumer Usage
- ToxCast in Vitro Data
- Exposure
- Analytical
- PubChem

- Summary
- Solubility
- Melting Point
- Boiling Point

LogP			
	Average	Median	Range
Experimental	1.19 (2)	1.19	1.19
Predicted	1.33 (3)	1.41	1.13 to 1.44

- CSV
- Excel

- LogP**
- Atmospheric Hydroxylation Rate
 - LogBCF
 - Biodegradation Half-life
 - Henry's Law Constant
 - Fish Biotransformation Half-life
 - LogKOA
 - LogKOC
 - Vapor Pressure

Experimental		
Source	Result	
EPI SUITE	1.19	-
CURATED PHYSPROP	1.19	-
Predicted		
Source	Result	Calculation Details
EPI SUITE	1.13	
ACD/Labs	1.44	
NCCT Models	1.41	

Calculation Details
 link to reports for
 T.E.S.T data and
 NCCT_Models

In vitro DB...

[Chemical Properties](#)

[External Links](#)

[Synonyms](#)

[Consumer Usage](#)

[ToxCast in Vitro Data](#)

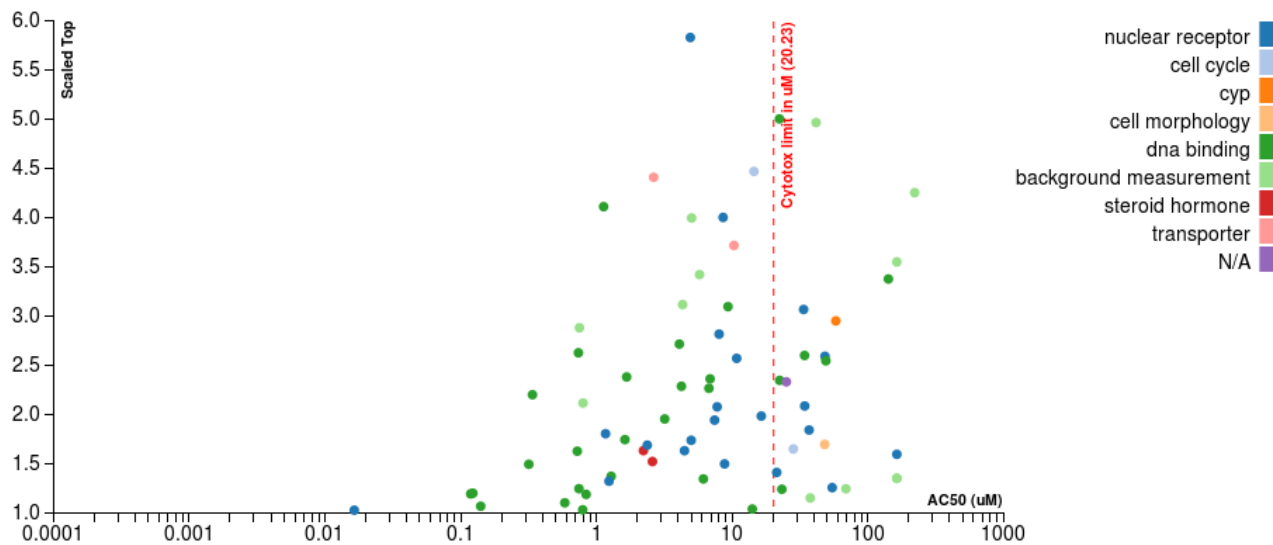
[Exposure](#)

[Analytical](#)

[PubChem](#)

[Comments](#)

Chemical Activity Summary



Assay Name	Hit Call	Top	Scaled Top	AC50	log AC50	Intended Target Family
ATG_TRANS	ACTIVE	1.680	1.419	21.317	1.329	nuclear receptor
TOX21_AR_BLA_Antagonist	ACTIVE	98.040	2.086	7.763	0.890	nuclear receptor

Consumer Usage (CPCat)

[Chemical Properties](#)

[External Links](#)

[Synonyms](#)

Consumer Usage

[ToxCast in Vitro Data](#)

[Analytical](#)

[Toxicity Values](#)

[PubChem](#)

[Comments](#)

Frequent Uses and Functions



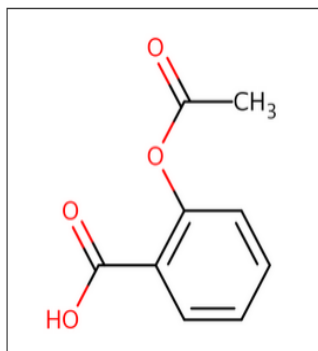
Product Composition

Product	Percent Composition	Manufacturer
CALCOZINE AURAMINE 00		AMERICAN CYANAMID CO
B604 AURAMINE O (C I 41000)		J T BAKER INC
AURAMINE O, B604	90-100%	J T BAKER INC
TB AURAMINE RHODAMINE T 3317	1.2%	DIFCO LABORATORIES, INC.
RET-SEARCH DYE/REC-800		SYSMEX

Calculation Details

Aspirin

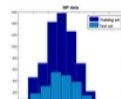
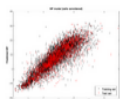
50-78-2 | DTXSID5020108



NCCT Models: LogP

Save Report

Model Performance



Weighted KNN model
15 molecular descriptors

OMRF

5-fold CV (75%)		Training (75%)		Test (25%)		
Q2	RMSE	N	R2	RMSE	N	R2
0.72	51.8	6486	0.74	50.27	2167	0.73

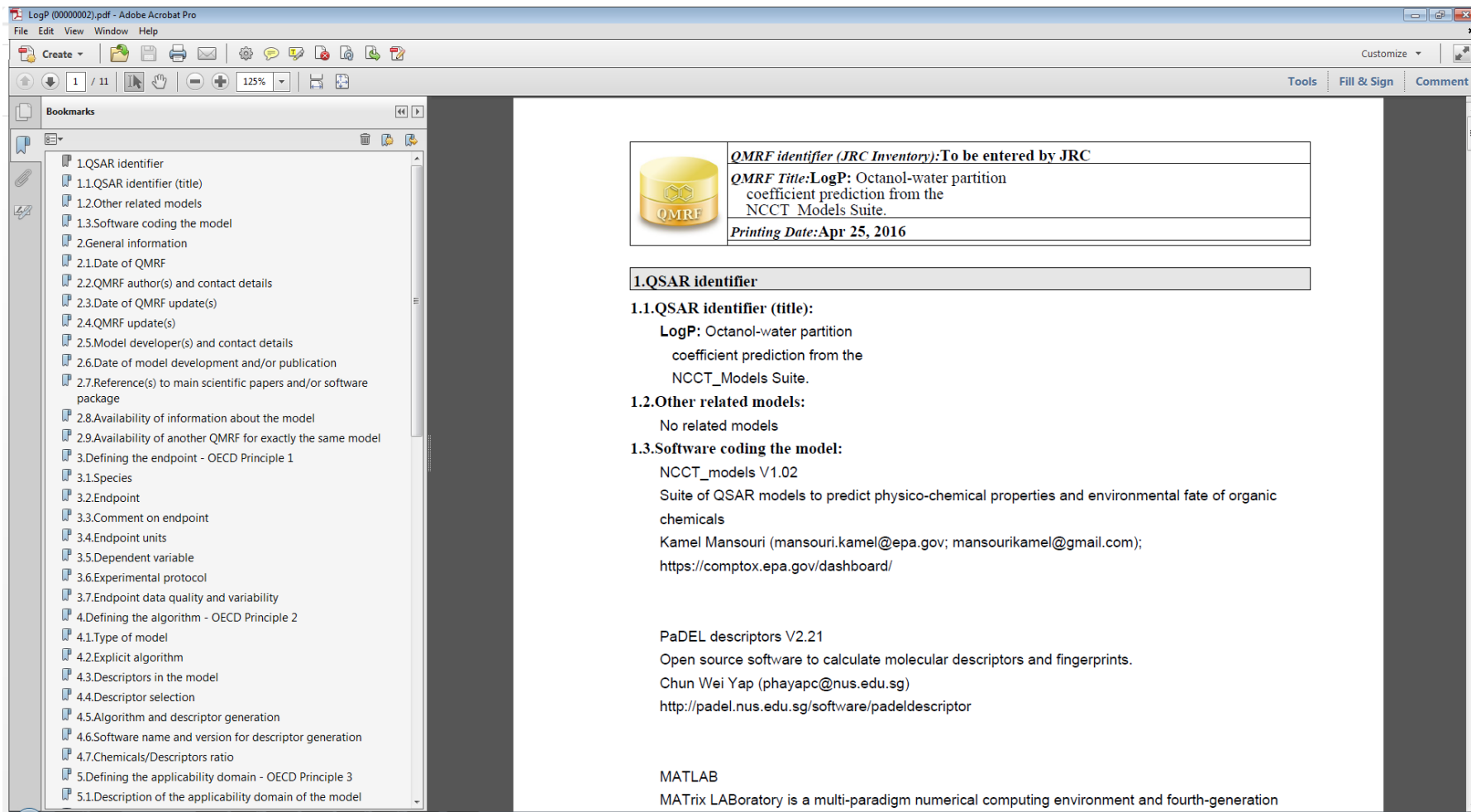
Model Results


Predicted value: 143°C
 Chemical in Training Set? No
 Global applicability domain: Inside ⓘ
 Local applicability domain index: 0.88 ⓘ
 Confidence level: 0.70 ⓘ

5 nearest neighbors from the training set

Observed Values:	20.1	20.1	20.1	20.1	20.1
Predicted Values:	30.7	30.7	30.7	30.7	30.7

DEVELOPMENT



	QMRF identifier (JRC Inventory): To be entered by JRC
	QMRF Title: LogP: Octanol-water partition coefficient prediction from the NCCT Models Suite.
	Printing Date: Apr 25, 2016

1. QSAR identifier

1.1. QSAR identifier (title):
LogP: Octanol-water partition coefficient prediction from the NCCT_Models Suite.

1.2. Other related models:
 No related models

1.3. Software coding the model:
 NCCT_models V1.02
 Suite of QSAR models to predict physico-chemical properties and environmental fate of organic chemicals
 Kamel Mansouri (mansouri.kamel@epa.gov; mansourikamel@gmail.com);
<https://comptox.epa.gov/dashboard/>

PaDEL descriptors V2.21
 Open source software to calculate molecular descriptors and fingerprints.
 Chun Wei Yap (phayapc@nus.edu.sg)
<http://padel.nus.edu.sg/software/padeldescriptor>

MATLAB
 MATrix LABORatory is a multi-paradigm numerical computing environment and fourth-generation

Toxicity Estimation Software Tool (TEST)

On this page:

- [QSAR Methodologies](#)
- **New!** [What's New in Version 4.2?](#)
- [Prior Version History](#)
- [System Requirements](#)
- [Installation Instructions](#)

The software includes models for the following endpoints:

- 96-hour fathead minnow 50 percent lethal concentration ([LC50](#))
- 48-hour daphnia magna 50 percent lethal concentration ([LC50](#))
- Tetrahymena pyriformis 50 percent growth inhibition concentration ([IGC50](#)) [Exit](#)
- Oral rat 50 percent lethal dose ([LD50](#)) [Exit](#)
- Bioconcentration Factor ([BCF](#)) The bioconcentration factor data set was compiled by researchers at the [Mario Negri Istituto Di Ricerche Farmacologiche](#) [Exit](#)
- Developmental Toxicity ([DevTox](#)) [Exit](#)
- Ames Mutagenicity ([Mutagenicity](#)) [Exit](#)

Subset of T.E.S.T Reports




Predicted Water solubility at 25°C for 75-05-8 from Consensus method

Prediction results

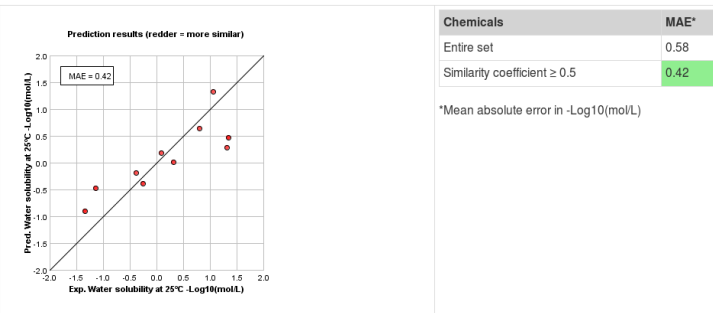
Endpoint	Experimental value (CAS= 75-05-8) Source: EPI Suite v 4.00	Predicted value ^a
Water solubility at 25°C -Log10(mol/L)	-1.39	0.06
Water solubility at 25°C mg/L	1000965.12	35541.38


^aNote: the test chemical was present in the training set. The prediction does not represent an external prediction.

Individual Predictions		Test chemical
Method	Predicted value -Log10(mol/L)	
Hierarchical clustering	N/A	
Group contribution	0.34	
Nearest neighbor	-0.21	

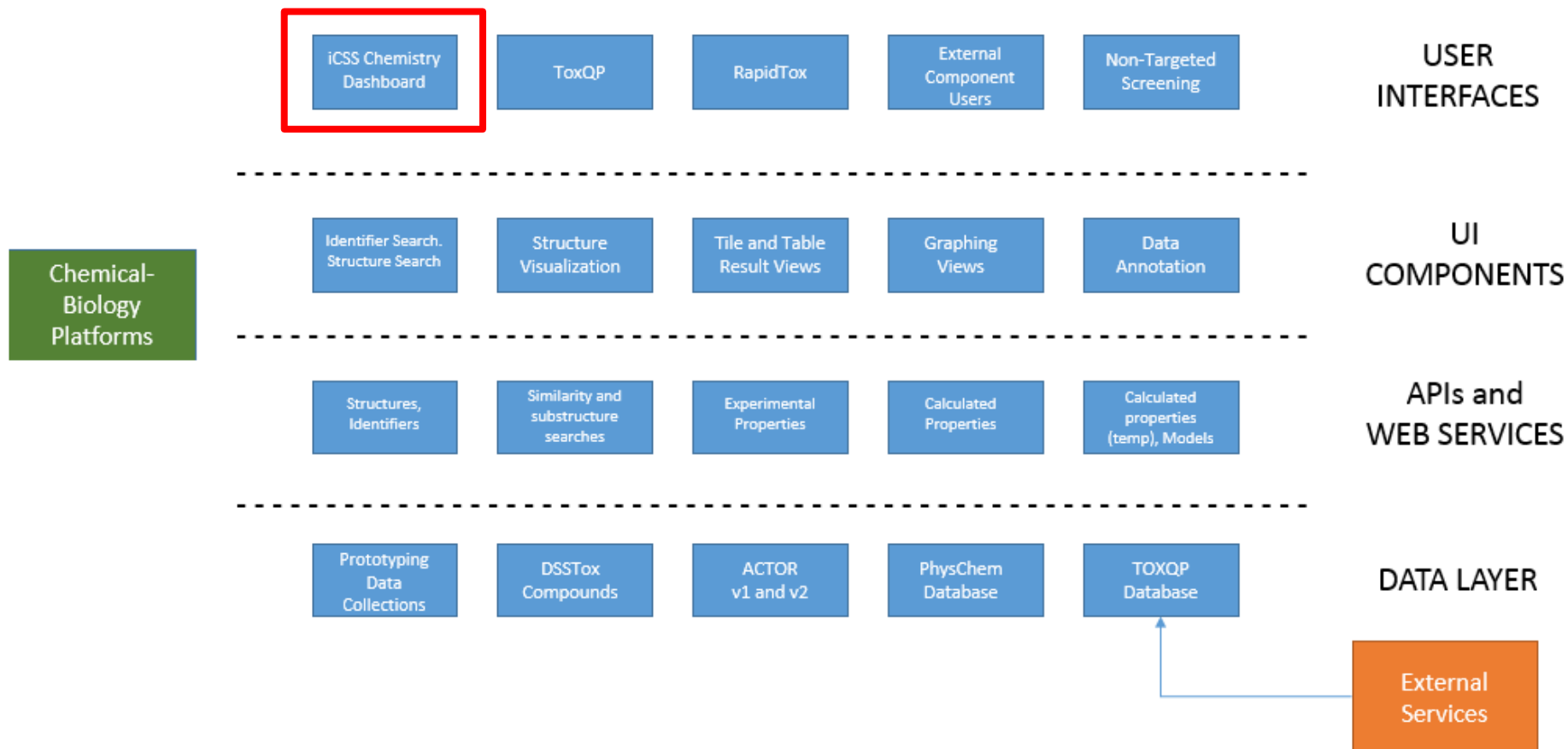
Predictions for the test chemical and for the most similar chemicals in the external test set

If *similar* test set chemicals were predicted well relative to the entire test set, one has greater confidence in the predicted value.



CAS	Structure	Similarity Coefficient	Experimental value -Log10(mol/L)	Predicted value -Log10(mol/L)
75-05-8 (test chemical)			-1.39	0.06
64-17-5	<chem>CCO</chem>	0.92	-1.34	-0.91
353-36-6	<chem>CCF</chem>	0.92	1.35	0.48

Chemistry Software Architecture



Summary

- iCSS Chemistry Dashboard has been in public *beta* for 2 months. Version 1 release scheduled for June 2016
- Validation of developing cheminformatics architecture
- Future Work:
 - Provide programmatic access to ORD data and algorithms
 - Integrate more ORD resources – e.g. ECOTOX, T.E.S.T
 - Integrate additional data resources
 - Integrate with NCCT applications
 - Support for chemical substances without structures
 - Continue to enhance our “***build once, use many***” architecture

Acknowledgments



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