

# Informatics Approaches for Developing and Organizing Chemical Descriptors

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Center for Computational Toxicology and Exposure Office of Research and Development U.S. Environmental Protection Agency

> Applying Exposure New Approach Methodologies to Chemical Risk Evaluation

International Society of Exposure Science

**September 21, 2020** 

The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA

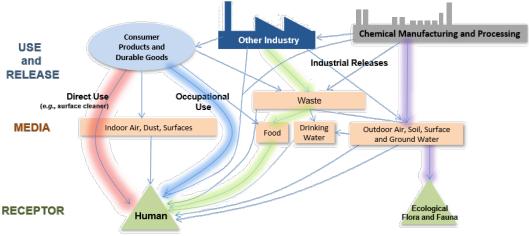


**Progress for a Stronger Future** 

https://orcid.org/0000-0001-9547-1654



- How do we 'parameterize' exposure models for different pathways?
- In some cases may only know chemical structure.
- Critical information:
  - How and how much chemical mass is applied, used, or released
  - Physical chemical properties
- Chemical information should ideally be organized in a in a machine-readable format.



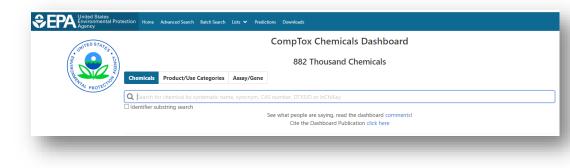
Exposure Pathway Classes: Consumer Occupational Ambient Ecological



# The CompTox Chemicals Dashboard

- Delivers *high-quality, structure-curated, open data* to meet the various needs of the environmental sciences and computational toxicology communities
- Provides intrinsic property, toxicity, and exposure data for chemicals, in addition to tools supporting:
  - Chemical similarity analyses
  - Read-across of chemical toxicity
  - Real-time property modeling
  - Identification of chemicals in mass spectrometry
  - Literature searching and identification of other information resources
- 10<sup>th</sup> Release (July 2020): 882,000 chemicals

#### https://comptox.epa.gov/dashboard





#### Open Access

# The CompTox Chemistry Dashboard: a community data resource for environmental chemistry

Antony J. Williams<sup>1\*</sup>, Christopher M. Grulke<sup>1</sup>, Jeff Edwards<sup>1</sup>, Andrew D. McEachran<sup>2</sup>, Kamel Mansouri<sup>1,2,4</sup>, Nancy C. Baker<sup>3</sup>, Grace Patlewicz<sup>1</sup>, Imran Shah<sup>1</sup>, John F. Wambaugh<sup>1</sup>, Richard S. Judson<sup>1</sup> and Ann M. Richard<sup>1</sup>

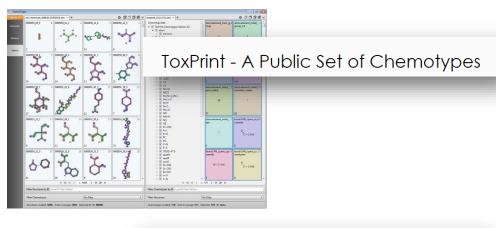


### **Chemical Descriptors in the Dashboard**

Molecular substructures

 Predicted EPA physical-chemical property data: Open Structure-Activity Relationship App ("OPERA")

 New descriptors containing information about *chemical use*





#### https://github.com/kmansouri/OPERA

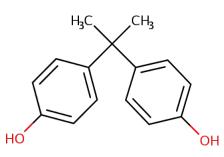


# **Chemical Property Descriptors in the Dashboard**

United States Environmental Protection Agency

- Chemical information may be reported using a many different chemical identifiers
  - Different names
  - Regional spellings/ different languages
  - Multiple standard identifiers, e.g. active or retired Chemical Abstract Registration Numbers (CASRN), Beilstein Registry Number

#### **Bisphenol A**

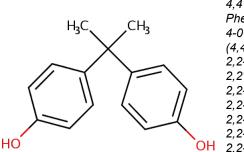




# How Do We Deal with Chemical Synonomy?

- Chemical information may be reported using a many different chemical identifiers
  - Different names
  - Regional spellings/ different languages
  - Multiple standard identifiers, e.g. active or retired Chemical Abstract Registration Numbers (CASRN), Beilstein Registry Number

#### **Bisphenol A**



Phenol, 4,4'-(1-methylethylidene)bis-80-05-7 BPA 4,4'-Propane-2,2-diyldiphenol Phenol, 4,4'-(1-methylethylidene)bis-4-06-00-06717 (4.4'-Dihydroxydiphenyl)dimethylmethane 2,2-Bis(4'-hydroxyphenyl) propane 2,2'-Bis(4-hydroxyphenyl)propane 2,2-BIS-(4-HYDROXY-PHENYL)-PROPANE 2,2-Bis(4-hydroxyphenyl)propane 2.2-Bis(p-hydroxyphenyl)propane 2,2-Di(4-Hydroxyphenyl) Propane 2,2-DI(4-HYDROXYPHENYL)PROPANE 2.2-Di(4-phenylol)propane 4,4'-(1-Methylethylidene)bisphenol 4,4'-Bisphenol A 4,4'-DIHYDROXYPHENYL-2,2-PROPANE 4,4'-isopropilidendifenol 4,4'-Isopropylidendiphenol 4,4'-Isopropylidene bisphenol 4,4-ISOPROPYLIDENE DIPHENYL 4,4'-Isopropylidenebis[phenol] 4,4'-isopropylidenediphenol 4,4'-Methylethylidenebisphenol Bis(4-hydroxyphenyl)dimethylmethane Bis(p-hydroxyphenyl)propane

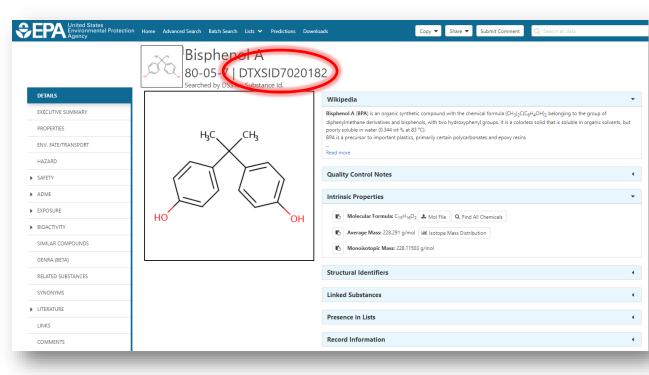
4,4'-(Propane-2,2-diyl)diphenol

#### +100 more



#### **DSSTox Substance Identifiers**

- The Dashboard provides a unique DSSTox Substance Identifier (DTXSID) for each chemical
- Also provides a preferred name and CASRN
- DTXSIDs are unique substance identifiers, where a substance can be any single chemical, mixture, polymer
- Linked to unique chemical structures (DTXCIDs)
- Can be obtained for lists of chemicals using the Dashboard's Batch Search Utility (tutorial later)

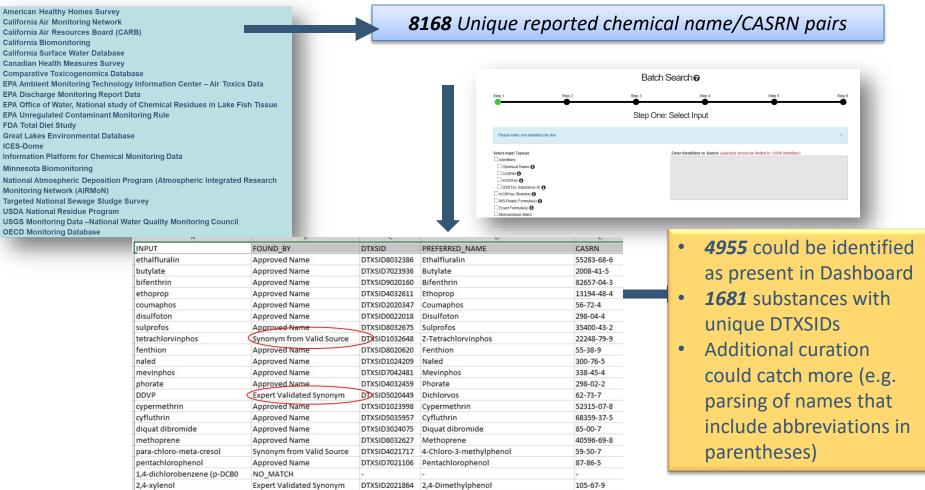




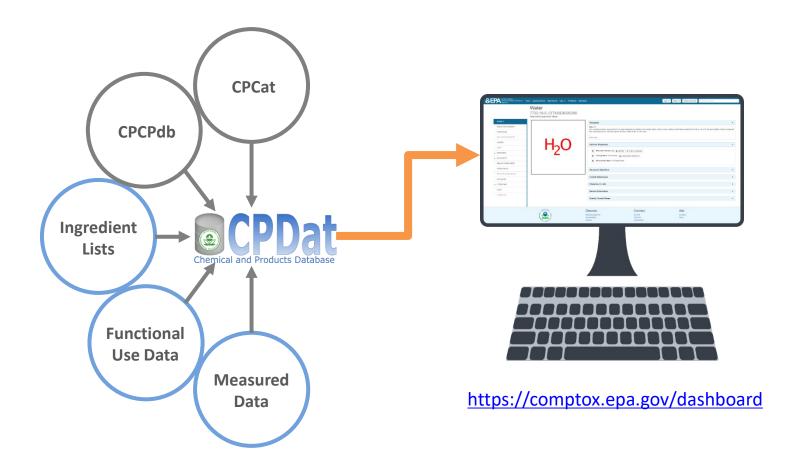
# Example of Harmonizing Messy Chemical Identifier Data

# We recently curated chemical identifiers from 20 public biomonitoring and environmental surveillance

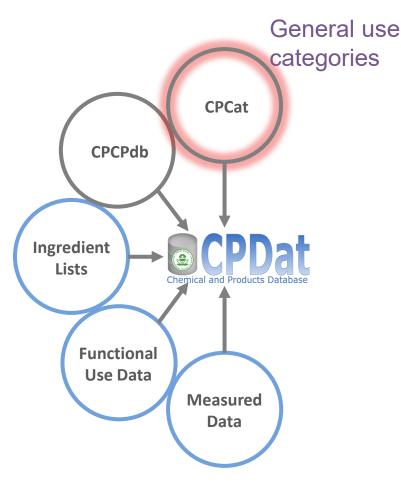
#### data sources







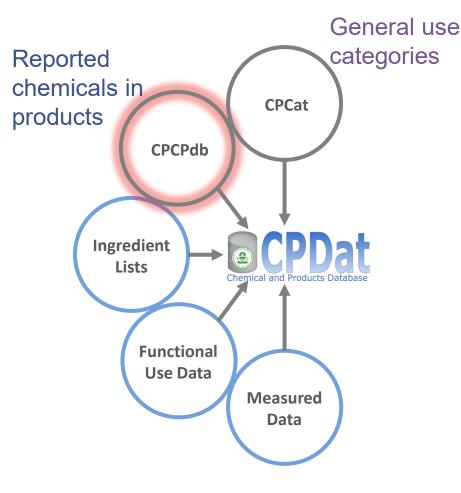






- Presence on other chemical lists
- Broad categorization of chemical use
  - Functional use
  - Therapeutic use
  - Consumer product-based use
  - Industrial process use
- Curated to a large number of relevant index terms

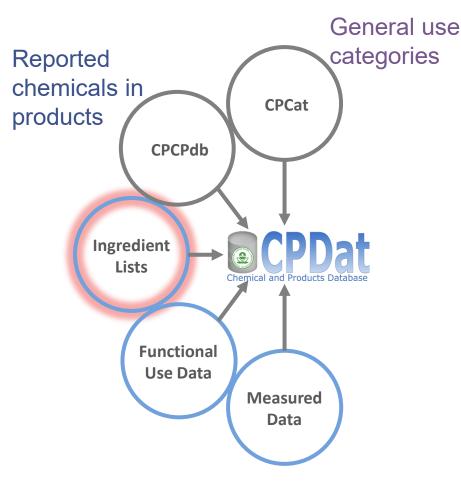






- MSDS-based composition information for consumer product formulations
  - Includes range of reported weight fraction
  - Provides quantitative input to consumer exposure models





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#### ORIGINAL ARTICLE

Consumer product chemical weight fractions from ingredient lists

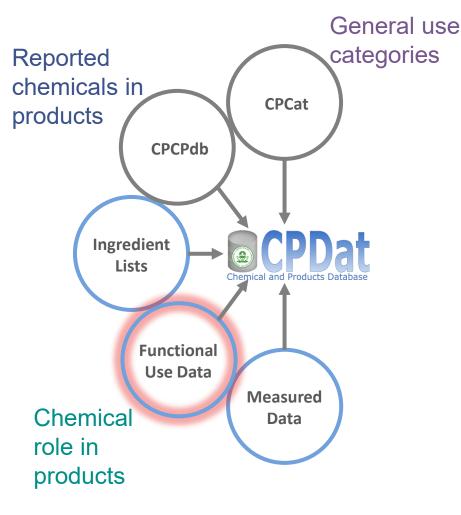
Kristin K. Isaacs<sup>1</sup>, Katherine A. Phillips<sup>1</sup>, Derya Biryol<sup>1,2</sup>, Kathie L. Dionisio<sup>1</sup> and Paul S. Price<sup>1</sup>

Assessing human exposures to chemicals in consumer products requires composition information. However, comprehensive composition data for products in commerce are not generally available. Many consumer products have reported ingredient lists that are constructed using specific guidelines. A probabilistic model was developed to estimate quantitative weight fraction (WF) values that are constructed using specific guidelines. A probabilistic model was developed to estimate quantitative weight fraction (WF) values that are consistent with the rank of an ingredient in the list, the number of reported ingredients of any rank in lists of any length. WFs predicted by the model compared favorably with those reported on Material Safety Data Sheets. Predictions for characterizes were also found to reasonably agree with reported WFs. The model was applied to a selection of publicly available ingredient lists, thereby estimating WFs for 1293 unique ingredients in 1123 products in 81 product categories. Predicted WFs, although less precise than reported values, can be estimated for large numbers of product-chemical combinations and thus provide a useful source of data for high-throughput or screening-level exposure assessments.

Journal of Exposure Science and Environmental Epidemiology advance online publication, 8 November 2017; doi:10.1038/jes.2017.29

- Keywords: consumer products; consumer exposures; ExpoCast; ingredients
- Chemical composition of consumer products from ingredient lists
  - Reported ingredients
  - Predicted weight fractions based on structured reporting rules

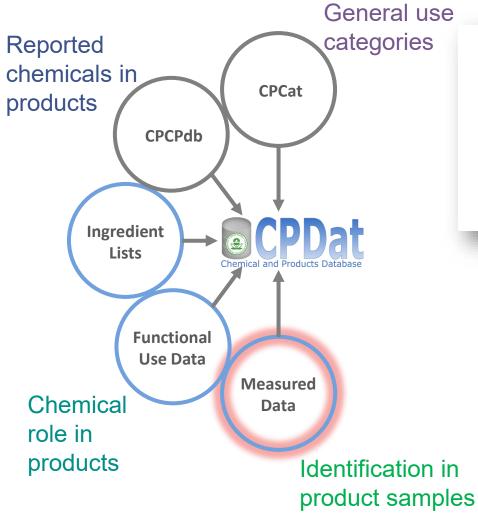






- Categorization by functional use
  - Reported functional use
  - Harmonized functional use
  - Predicted functional uses based on structure







#### Suspect Screening Analysis of Chemicals in Consumer Products

Katherine A. Phillips,<sup>†</sup><sup>●</sup> Alice Yau,<sup>‡</sup> Kristin A. Favela,<sup>‡</sup> Kristin K. Isaacs,<sup>†</sup> Andrew McEachran,<sup>§,||</sup> Christopher Grulke,<sup>||</sup> Ann M. Richard,<sup>||</sup> Antony J. Williams,<sup>||</sup> Jon R. Sobus,<sup>†</sup> Russell S. Thomas,<sup>||</sup> and John F. Wambaugh<sup>\*,.||</sup>

<sup>†</sup>National Exposure Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, 109 T. W. Alexander Drive, Research Triangle Park, North Carolina 27711, United States

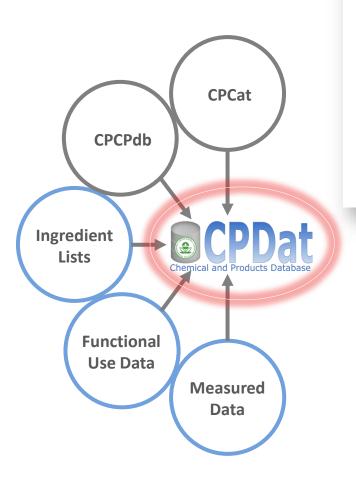
<sup>‡</sup>Southwest Research Institute, San Antonio, Texas 78238, United States

<sup>§</sup>Oak Ridge Institute for Science and Education (ORISE), Oak Ridge, Tennessee 37830, United States

<sup>II</sup>National Center for Computational Toxicology, Office of Research and Development, U.S. Environmental Protection Agency, 109 T. W. Alexander Drive, Research Triangle Park, North Carolina 27711, United States

- Targeted and non-targeted measurement of chemicals in consumer products
  - Measured weight fractions
  - Confirmed presence
  - Tentative identification





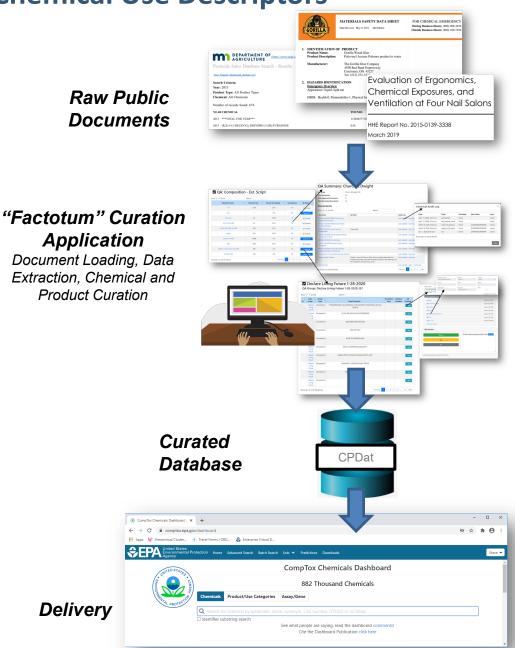


- Broad categorization of chemical use
- Comprehensive hierarchical categorization of chemical usage by consumer product type
- Functional use of chemicals
- Quantitative chemical composition for consumer products



## **Curation of Chemical Use Descriptors**

- We are using informatics approaches to obtain and curate additional chemical descriptor information
- Data from chemical use, monitoring, and release domains
- Public data sources: reports, open literature, databases
- Utilizing standard curation/QA procedures and tools



https://comptox.epa.gov/dashboard



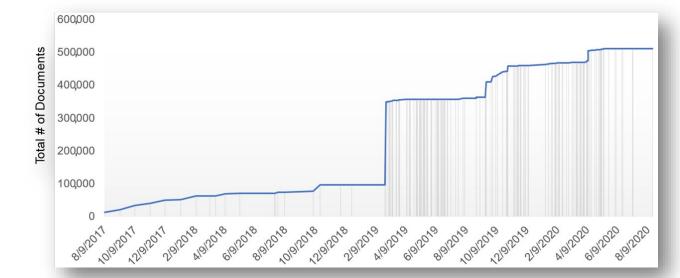
Number of

2020

Documents in

Factotum 2017-

### **Chemical Descriptor NAMs**



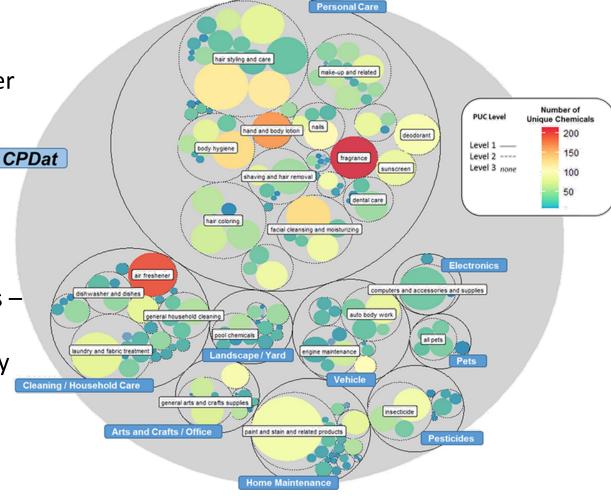
Group Type	Documents	Raw Chemical Records	Curated Chemical Records
Consumer Product	473,271	3,738,350	1,791,250
Composition			
Functional use	33,770	34,680	11,946
CPCat Categories	2,088	117,231	68,133
Occupational exposure	1,304	4,825	1078
Literature monitoring	1,175	966	In process
Habits and practices	202	NA	NA

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# **Product categories in Factotum/CPDat**

- Allows for linking to consumer product exposure models
- Maps to habits and practices data
- Maps to exposure algorithms if chemical and product are known, models can be rapidly and parameterized





## **Curation of Products to Consumer Product Categories**

- Machine learning classifiers were built using the existing manually curated CPDat data as a training set
- Allowed for automated curation of new documents to Product Use Categories (PUCs) developed specifically for consumer exposure modeling.



New Product Data Documents (Safety Data Sheets (SDS, Ingredient lists, ingredient disclosures)

CPDat Training set (15000+ product names linked to manually-assigned categories) One-Vs-Rest Support Vector Machine Classifiers

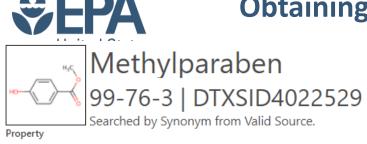
Automated assignment to Product Use Categories (PUCs, Isaacs et al. 2020)



SEPA United States Environmental Prote Agency	ection Home	Advanced Search	Batch Search	Lists 🗸	Predictions	Downloads
UNITED STATED					Co	ompTox Chemicals Dashboard
SUN NOR						882 Thousand Chemicals
ON THE PROTECTION	Chemicals	Product/Use	Categories	Assay/0	Sene	
	Q methyl p	araben				
	ldentifier su	bstring search				
	_	_			See v	what people are saving, read the dashboard comments!



DETAILS	Methylparaben 99-76-3   DTXSID402252 Searched by Synonym from Valid Source.	
		Wikipedia
PROPERTIES		Methylparaben, also methyl paraben, one of the parabens, is a preservative with the chemical formula $CH_3(C_6H_4(OH)COO)$ . It is the methyl ester of $p$ -hydroxybenzoic acid.
ENV. FATE/TRANSPORT	H <sub>3</sub> C	Read more
HAZARD		Quality Control Notes
► SAFETY		Intrinsic Properties
► ADME	HO	Molecular Formula: C <sub>8</sub> H <sub>8</sub> O <sub>3</sub> 📥 Mol File 🔍 Find All Chemicals
EXPOSURE		Average Mass: 152.149 g/mol ull Isotope Mass Distribution
BIOACTIVITY		Monoisotopic Mass: 152.047344 g/mol
SIMILAR COMPOUNDS		
GENRA (BETA)		Structural Identifiers
RELATED SUBSTANCES		Linked Substances
SYNONYMS		
► LITERATURE		Presence in Lists
LINKS		Record Information
COMMENTS		



Υ.

🛓 Download 🔻 🛛 Columns 🗸

Vapor Pressure

Search query

Property 🗘	Experimental average	Predicted average 🕈	Experimental median 🗘	Predicted median \$	Experimental range	Predicted range	Unit 🗘
LogKow: Octanol-Water	1.96 (1)	1.99		1.98	1.96	1.86 to 2.14	-
Melting Point	128 (9)	83.7	127	69.4	126 to 131	51.5 to 130	°C
Boiling Point	278 (3)	261	280	260	275 to 280	252 to 273	°C
Water Solubility	1.73e-2 (4)	1.23	1.66e-2	2.82e-2	1.64e-2 to 1.97e-2	1.22e-2 to 4.86	mol/L
Flash Point	-	115		115	-	113 to 116	°C
Density	-	1.20		1.20	-	1.20 to 1.21	g/cm^3
Vapor Pressure	-	4.98e-3		5.55e-3	-	1.08e-3 to 8.32e-3	mmHg
Thermal Conductivity	-	150			-	150	mW/(m*K)
Viscosity	-	7.03			-	7.03	cP
Surface Tension	-	42.3		42.3	-	38.7 to 45.8	dyn/cm
Index of Refraction	-	1.55			-	1.55	-
Molar Refractivity	-	39.9			-	39.9	cm^3
Polarizability	-	15.8			-	15.8	Å^3

Summary



EogKow: Octanol-Water ▼     LogKow: Octanol-Water     LogKow: Octanol-Water										
Type 🗘	Avera	age		\$	Median	\$	Range	\$	Unit	¢
Experimental	1.96				-		1.96		-	
Predicted	1.99				1.98		1.86 to 2.14		-	
Experimental Data Source						\$				
PhysPropNCCT			1.96							
Predicted										
Source	\$	Result	\$	Calculat	ion Details		\$	QMRF		¢
EPISUITE		2.00	Not Available				Not Avai	able		
ACD/Labs Consensus		2.14	Not Available				Not Avail	able		
ACD/Labs		1.86		Not Avai	lable		Not Available		able	
OPERA		1.96		OPERA I	Model Report [Ins	de AD]		Available		



	🔄 🔩 Methylparaben		
	99-76-3   DTXSID402252 Searched by Synonym from Valid Source.	29	
DETAILS		Wikipedia	•
EXECUTIVE SUMMARY		$\textbf{Methylparaben}, also \textbf{methyl paraben}, one of the parabens, is a preservative with the chemical formula CH_3(C_6H_4(OH)COO). It is the the other than the the the the the the the the the the$	:he
PROPERTIES		methyl ester of <i>p</i> -hydroxybenzoic acid.	
ENV. FATE/TRANSPORT	H <sub>3</sub> C	Read more	
HAZARD		Quality Control Notes	•
► SAFETY		Intrinsic Properties	•
► ADME	HO	▶ Molecular Formula: C <sub>8</sub> H <sub>8</sub> O <sub>3</sub> 🕹 Mol File Q. Find All Chemicals	
► EXPOSURE			
BIOACTIVITY		Average Mass: 152.149 g/mol	
SIMILAR COMPOUNDS		Monoisotopic Mass: 152.047344 g/mol	
GENRA (BETA)		Structural Identifiers	4
RELATED SUBSTANCES		Linked Substances	•
SYNONYMS			
▶ LITERATURE		Presence in Lists	•
LINKS		Record Information	•
COMMENTS			



Methylparaben

Searched by Synonym from Valid Source.

99-76-3 | DTXSID4022529

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

EXPOSURE PREDICTIONS PRODUCTION VOLUME

HAZARD

SAFETY

ADME

EXPOSURE

ETAILS				
KECUTIVE SUMMARY	La Download    Columns    10			Search query
ROPERTIES				
NV. FATE/TRANSPORT	Product or Use Categorization	Categorization type \$	Number of Unique Products	\$
	hair styling and care:	PUC	1	
AZARD	hair styling and care: hair conditioner - leave-in	PUC	1	
AFETY	hair styling and care: hair conditioner	PUC	1	
DME	hair styling and care: hair styling	PUC	2	
XPOSURE	hair styling and care: lice shampoo	PUC	1	
	hair styling and care: shampoo	PUC	1	
PRODUCT & USE CATEGORIES	home office: pens and markers	PUC	2	
CHEMICAL WEIGHT FRACTION	inert_ingredient, Pesticides	CPCat Cassette	1	
CHEMICAL FUNCTIONAL USE	inert_ingredient, non_food_use, Pesticides	CPCat Cassette	1	
TOXICS RELEASE INVENTORY	make-up and related: eye liner	PUC	1	
MONITORING DATA	<< < 1	2 3 4 5 6 > >>		

Product and Use Categories (PUCs)

Showing 31 to 40 of 54 records

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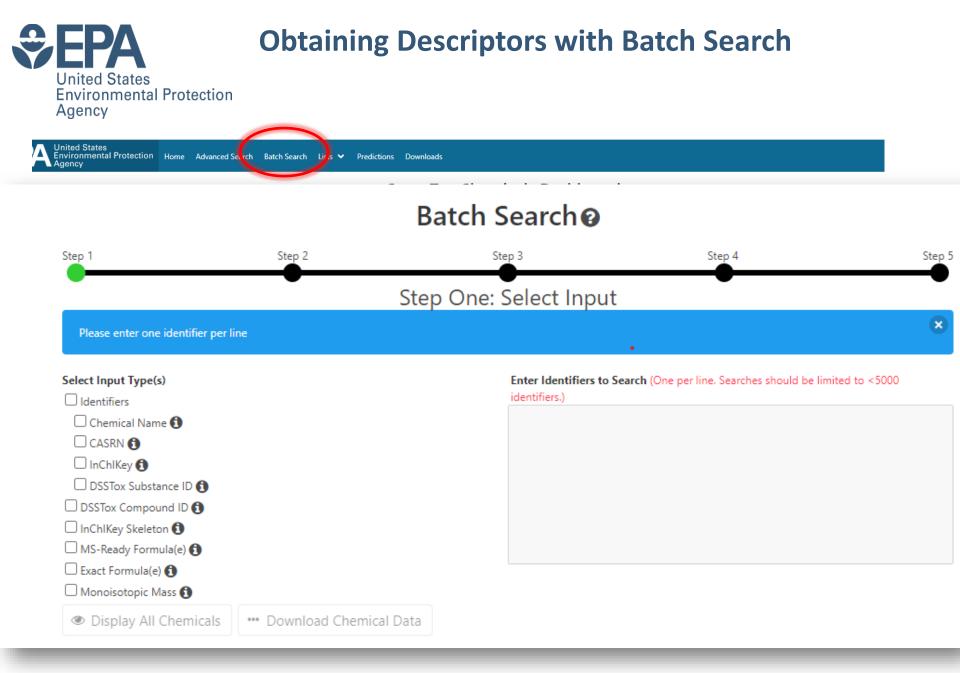


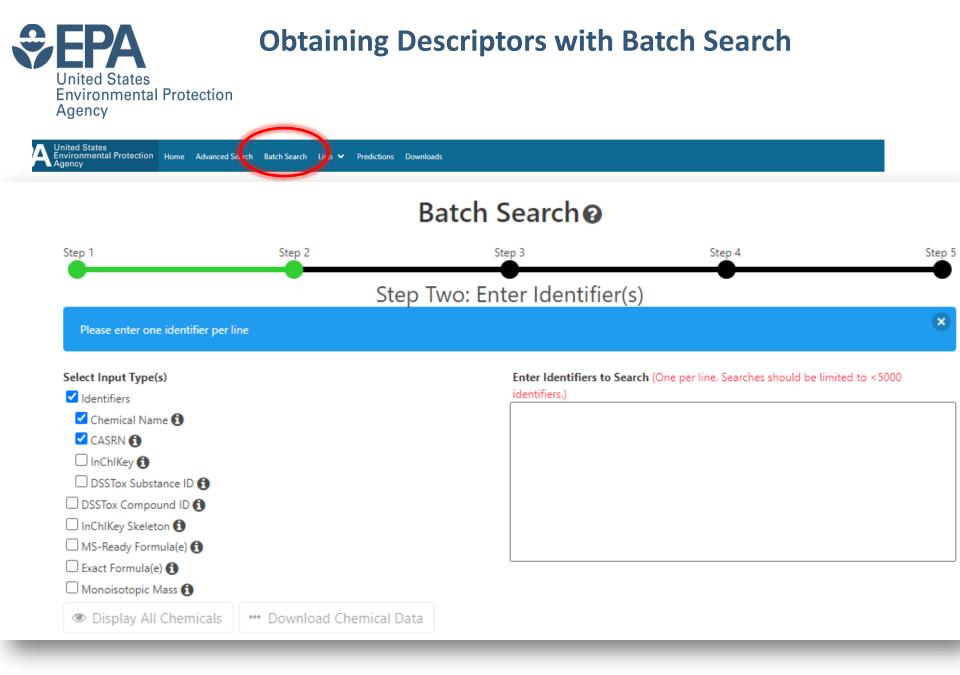
		Methylparaben 99-76-3   DTXSID4022529 Searched by Synonym from Valid Source.					
DETAILS Collected Data on Functional Use 🕦							
EX	ECUTIVE SUMMARY		Search query				
PR	OPERTIES						
EN	V. FATE/TRANSPORT	Harmonized functional use	\$	Reported functional use		\$	
		fragrance		fragrance			
HA	ZARD	fragrance		preservative			
► SA	FETY						
► AE	ME						
▼ EX	POSURE	Predicted Probability of Associated Functional Use <b>1</b> QSAR Version/Date: 2015-11-06					
	PRODUCT & USE CATEGORIES	QSAR Versio	n/Dat	e: 2015-11-06			
	CHEMICAL WEIGHT FRACTION	La Download   10   10     10				Search query	
	CHEMICAL FUNCTIONAL USE	Harmonized functional use		\$	Probability	\$	
	TOXICS RELEASE INVENTORY	preservative			0.988		
	MONITORING DATA	uv_absorber			0.885		
		antioxidant			0.733		
	EXPOSURE PREDICTIONS	skin_conditioner			0.661		
	PRODUCTION VOLUME	fragrance			0.567		
► BI	DACTIVITY	skin_protectant			0.457		
SI	AILAR COMPOUNDS	chelator			0.364		
	NDA (DETA)	colorant			0.291		

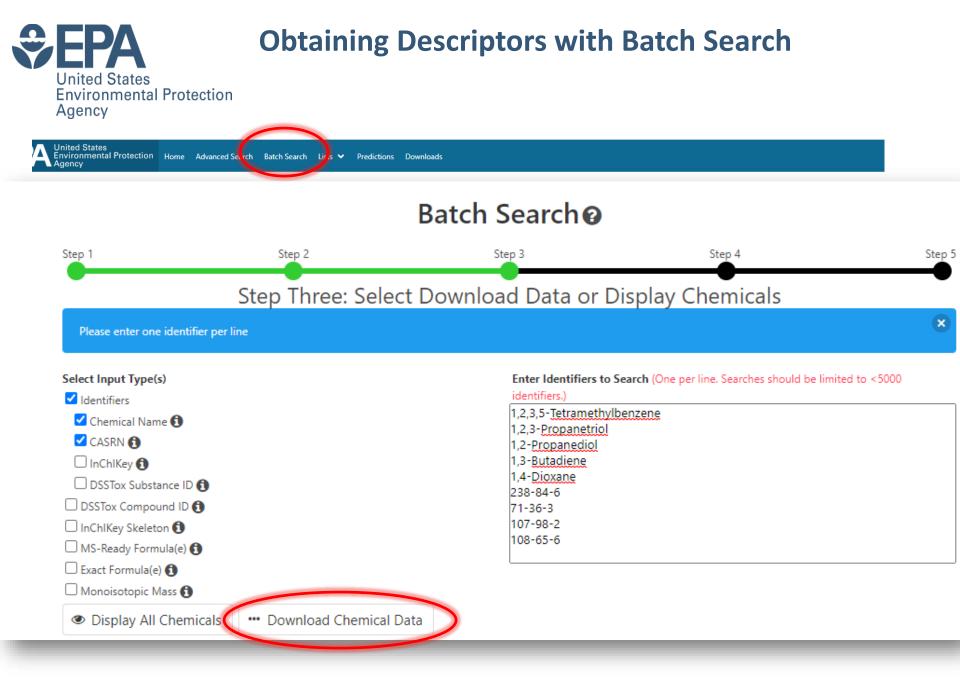


		Methylparaben 99-76-3   DTXSID4022529 Searched by Synonym from Valid Source.					
DETAILS Collected Data on Functional Use 🕦							
EX	ECUTIVE SUMMARY		Search query				
PR	OPERTIES						
EN	V. FATE/TRANSPORT	Harmonized functional use	\$	Reported functional use		\$	
		fragrance		fragrance			
HA	ZARD	fragrance		preservative			
► SA	FETY						
► AE	ME						
▼ EX	POSURE	Predicted Probability of Associated Functional Use <b>1</b> QSAR Version/Date: 2015-11-06					
	PRODUCT & USE CATEGORIES	QSAR Versio	n/Dat	e: 2015-11-06			
	CHEMICAL WEIGHT FRACTION	La Download   10   10     10				Search query	
	CHEMICAL FUNCTIONAL USE	Harmonized functional use		\$	Probability	\$	
	TOXICS RELEASE INVENTORY	preservative			0.988		
	MONITORING DATA	uv_absorber			0.885		
		antioxidant			0.733		
	EXPOSURE PREDICTIONS	skin_conditioner			0.661		
	PRODUCTION VOLUME	fragrance			0.567		
► BI	DACTIVITY	skin_protectant			0.457		
SI	AILAR COMPOUNDS	chelator			0.364		
	NDA (DETA)	colorant			0.291		

United Sta Environme Agency	Obtaining Descriptors with Batch Search	
United States Environmental Prot Agency	Home       Advanced Serich       Batch Search       Lips       Predictions       Downloads         CompTox Chemicals Dashboard         882 Thousand Chemicals         Chemicals         Product/Use Categories       Assay/Gene	
	Q search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey         Identifier substring search         See what people are saying, read the dashboard comments!         Cite the Dashboard Publication click here	









Batch Search@ Step 3 Step Five: Click "Download" Select Input Type(s) Enter Identifiers to Search (One per line. Searches should be limited to <5000 identifiers.) 1,2,3,5-Tetramethylbenzene Identifiers 1.2.3-Propagetriol Chemical Name 1,2-Propanediol 1,3-Butadiene CASRN 6 InChikey 1.4-Dioxane 238-84-6 DSSTox Substance ID 71-36-3 DSSTax Compound ID 107-98-2 InChiKey Skeleton 108-65-6 MS-Ready Formula(e) Exact Formula(e) Monoisotopic Mass Display All Chemicals
 "" Download Chemical Data Select Output Format: Excel ~ A Download Customize Results Presence in Lists: Select All 40CFR116.4 Designation of Hazardous Substances (Above Ground Storage Tanks) Select All in Lists 40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities 🖉 Chemical Identifiers AEGLS: Acute Exposure Guideline Levels 🕝 DTXSID 🚯 ANDROGEN: Androgen Receptor Chemicals 🕑 Chemical Name ARTICLE: Bench-Mark Dose Human Health Assessment List (Wignall et al. 2014) ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (CERAPP) CAS-RN () ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (COMPARA) InChilKey () ATSDR: Minimal Risk Levels (MRLs) for Hazardous Substances 3 UIUPAC Name ATSDR: Toxic Substances Portal Chemical List 🕑 Structures California Office of Environmental Health Hazard Assessment 🕈 Mol File A Canadian Domestic Substances List 2019 3 Chemicals in human blood (plasma and serum) 🕑 InChi String CHEMINV; ToxCast/Tox21 Chemical inventory available as DMSO solutions (20181123) MS-Ready SMILES CHEMINV: EPA Chemical Inventory for ToxCast 3 QSAR-Ready SMILES Intrinsic And Predicted Propertie CHEMINV: EPA ToxCast CHEMINV list of volatiles CHEMINV: EPA ToxCast Cheminventory chemicals with stability problems 3 Molecular Formula CHEMINV: EPA ToxCast Cheminventory DMSO Insolubles Average Mass 🚯 CHEMINV: EPA ToxCast Cheminventory List of Reactives 🧭 Monoisotopic Mass () TEST Model Predictions Consolidated List of Lists under EPCRA/CERCLA/CAA \$112(r) (June 2019 Version) COSMOS DB cosmetics database 🕑 OPERA Model Predictions Metadata DRUGS >8600 Pharmaceuticals from ZINC15 C Curation Level Details 🗆 DRUGS: Antibiotics 🗹 NHANES/Predicted Exposure DRUGS: DrugBank database from the University of Alberta 🧭 Data Sources () DRUGS: ITNANTIBIOTIC list of antibiotics C Include ToxVal Data Availability DRUGS: List of opioids and related metabolites 🕑 Assay Hit Count () DRUGS: Pharmaceutical List with EU, Swiss, US Consumption Data 🗭 Number of PubMed Articles 🗆 DRUGS: Statin drugs 🗷 PubChem Data Sources DRUGSINORMAN: Target Pharmaceutical/Drug List from University of Athens CPDat Product Occurrence Count 🚯 DRUGS/WIKILIST: Veterinary Drugs 🖉 E-LIQUIDS DB Center for Tobacco Regulatory Science and Lung Health UNC PPRTV () ECOTOX: Ecotoxicology knowledgebase Wikipedia Article ENDOCRINE: EDSP Universe of Chemicals OC Notes ENDOCRINE: EDSP21 Tier 1 Screening Chemicals: List 1 3 Include links to ACToR reports - SLOWI (BETA) ENDOCRINE: EDSP21 Tier 1 Screening Chemicals: List 2 🕑 Enhanced Data Sheets EPA HTPP Reference Set - Nyffeler et al. 2019 MetFrag Input File (Beta) EPA HTPP Screening Set - Nyffeler et al. 2019 ToxPrint single fingerprints () EPA Regional Screening Levels Data Chemicals List 🧭 Abstract Sifter Input File (Beta) EPA: Chemicals mapped to HERO 🗷 Synonyms and Identifiers EPA: Superfund Chemical Data Matrix 🕜 Related Substance relationships EPA: Constituents Of Motor Fuels Relevant To Leaking Underground Storage Tanks 🧭 ToxPrint fingerprints (ChemoTyper format - CSV/TSV only) Associated ToxCast Assays EPA: Consumer Products Suspect Screening Result C EPA: CPDAT, Chemical and Products Database 🗆 EPA: Hazardous waste P & U Lists 🗭 EPA: High Production Volume List EPA: IRIS Chemicals EPA: List of solvents in the PARIS III Solvent Database EPA: Mechanism of Action (MoA) for aquatic toxicity EPA: National-Scale Air Toxics Assessment (NATA) EPA: PPRTV Chemical Report 🧭 EPA: Provisional Advisory Levels (Inhalation) EPA: Provisional Advisory Levels (Oral) EPA: Toxicity Values Version 5 (Aug 2018) EPA: Toxics Release Inventory 🧭 EPA: Underground Storage Tanks (USTs) EPAJECOTOX: Fathead Minnow Acute Toxicity

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#### Opens large panel of available chemical data for selection



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PPRTV 🚯	ECOTOX: Ecotoxicology knowledgebase     C				
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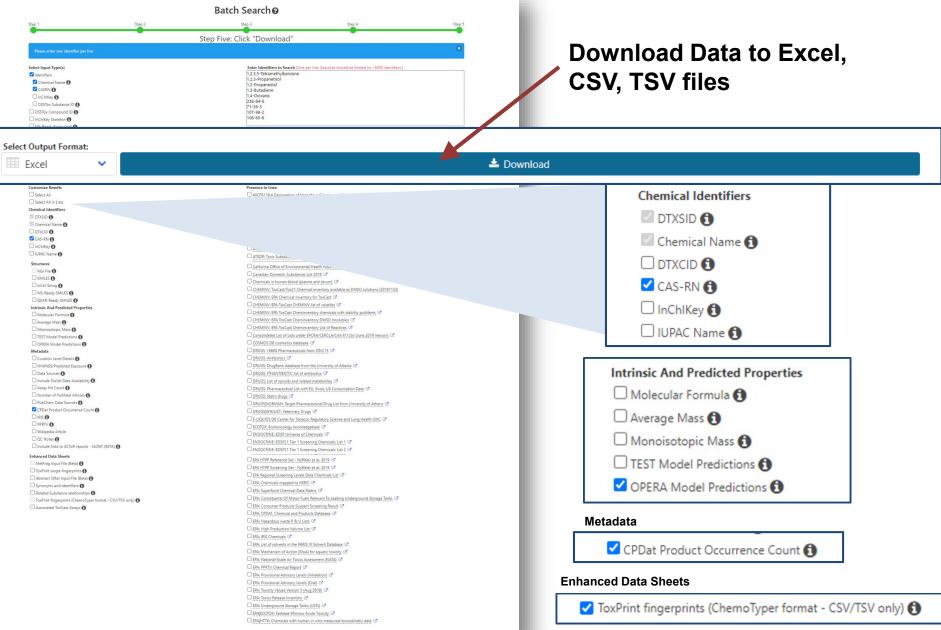
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#### Downloaded File Contains Original Identifier, DTXSID, and selected datasets

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1 INPUT	FOUND_BY	DTXSID	PREFERRED_NAME	CASRN	CPDAT_COUNT		BIOCONCENTR/ BIO					
			1,2,3,5-Tetramethylbenzer		-	2.60907E-11	106.447	3.0043	199.912	0.0077477		
3 1,2,3-Propanetric				56-81-5	24981		2.72028	5.37604	289.982	1.72905E-08		
			1,2-Propylene glycol	57-55-6	25776		3.38004	4.268	187.669	6.05478E-08		
5 1,3-Butadiene	Approved Name			106-99-0	249		11.0393	7.46888	-4.28507	0.0412947		
6 1,4-Dioxane				123-91-1	1185		0.505112	9.35852	101.605	4.89581E-06		
7 238-84-6			11H-Benzo[a]fluorene	238-84-6	1	1.99178E-11	678.84	140.966	404.821	2.65973E-05		
8 71-36-3		DTXSID1021740		71-36-3	14816		4.82036	4.43732	117.709	8.83859E-06		
9 107-98-2			1-Methoxy-2-propanol	107-98-2	2342		2.34662	4.27926	119.193	9.14241E-07		
10 108-65-6	CAS-RN	D1X5ID1026796	1-Methoxy-2-propyl acetat	e 108-65-6	8600	1.19667E-11	3.34681	4.28671	145.608	1.69436E-05	0.147463	5 4

# **ExpoCast Project** (Exposure Forecasting)

#### **CCTE**

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