

#### Exposure Data Available through EPA's CompTox Chemicals Dashboard

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#### Acknowledgements

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Kristin Isaacs **Richard Judson** Jen Korol-Bexell\* Anna Kreutz\* Charles Lowe\* Seth Newton Alli Phillips Katherine Phillips Paul Price Ann Richard Caroline Ring **Risa Sayre** Mark Sfeir\* Marci Smeltz\* Jon Sobus

Zach Stanfield\* Mike Tornero-Velez **Rusty Thomas** Elin Ulrich Dan Vallero Barbara Wetmore John Wambaugh Antony Williams

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## **Exposure Information in the Dashboard**

#### Outline

- Background and Motivation
- Types of Exposure information
  - -Collected
  - -Assigned
  - -Predicted
- How to get this information





### **Rapid Exposure and Dosimetry**





#### **Exposure Pathways**





### **Consensus Exposure Predictions**

- Different exposure models incorporate knowledge, assumptions, and data (MacLeod et al., 2010)
- We incorporate multiple models (including SHEDS-HT, ExpoDat) into consensus predictions for 1000s of chemicals within the Systematic Empirical Evaluation of Models (SEEM) (Wambaugh et al., 2013, 2014, Ring et al., 2019)
- Evaluation is like a sensitivity analysis: What models are working? What data are most needed?



Predicting Hurricane path from many models



Office of Research and Development Center for Computational Toxicology and Exposure



#### Predicting COVID-19 case loads from surveillance data and many models

Slide adapted from Kristin Isaacs and John Wambaugh Wambaugh et al., *Current Opinion in Toxicology*, 2019



# High-Throughput Exposure Models

- Information on Users
  - What products do they use?
  - What activities do they typically do?
  - What food do they eat?
- Information on Products
  - What compounds are intentionally added?
  - How much of a compounds is intentionally added?
  - What compounds are unintentionally added?
    - Reaction/degradation of intentionally added compounds
    - Contamination throughout supply chain
- Information on Chemicals





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Center for Computational Toxicology and Exposure



Factotum: Application for the storage, management, and curation of exposure factor data in CPDat

- Facilitates loading of large quantities of data into CPDat (raw documents and curated data)
- Allows for tracking of data provenance
- Provides tools for curating data
- Currently disseminates data to internal EPA users; external access in the future

#### Welcome to Factotum

Factorum is an application for storing and curating publicly-available documents containing information on how chemicals are used and how they occur in consumer and industrial products. Factorum provides tools for EPA users to explore and download these data and the original source documents, which include consumer product composition, chemical functional use, and general chemical use information. Factorum curators and developers actively work to curate these chemical data to harmonized chemical identifiers (DTXSIDs), product use categories (PUCs), and functional use categories.

Documents <b>552,747</b>	Products <b>701,601</b>	Products Linked To Product Use Categories <b>617,853</b>
Extracted Chemical Records	Curated Chemical Records	Unique Chemicals (DTXSIDs)
3.9 million	2.6 million	34,137



### Additional Collected Data from Dashboard





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### Product Use Categories

Products in CPDat are assigned product use categories (PUCs) which:

- Are hierarchical, allowing for aggregation up do a higher level
- Have attributes which allow for further specifications of products:
  - Form (e.g., spray, gel, foam, etc.)
  - Microenvironment (interior vs. exterior)
  - Population (adult vs. child)
  - One or two component product
- Bridge product information and both exposure modeling and chemical reporting

	Formulation PUCs	
	General Category - Product Family - Product Type	
Ø	Arts and crafts/office supplies 🕚	24891
Ø	Sports equipment 🕕	316
Ø	Cleaning products and household care 🕕	99350
Ø	Electronics/small appliances 🕕	20071
Ø	Home maintenance 🕕	132325
Ø	Landscape/yard 🕦	5641
Ø	Personal care 🕦	234243
Ø	Pesticides 🕕	7456
Ø	Pet care 🚯	3302
Ø	Vehicle 🕕	25779
Ø	Other consumer products ()	-
Ø	Food and drug 🚯	7951





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### **SEEM3 Considers Pathway of Exposure**

We organize models by the exposure pathways they cover

We calibrate predictors based on ability to explain median NHANES exposure rates

> General Population Median Chemical Exposure (mg/kg BW/day)



Slide from John Wambaugh Ring et al., *Environ. Sci. & Tech.*, 2018



- We predict relevant pathway(s), median intake rate, and credible interval for each of 479,926 chemicals
- Of 687,359 chemicals evaluated, 30% have low probability for exposure via any of the four pathways – they are considered outside the domain of applicability
- There is a 95% confidence that the median intake rate is below 1 mg/kg-BW/day for 474,572 compounds
- This 95% interval reflects confidence in the median estimate – not the most highly exposed individuals



Ring et al., Environ. Sci. & Tech., 2018



### Quantitative Structure-Use Relationships (QSURs)



additive	additive	rubber additive	adhesion promoter	antimicrobial	antioxidant	antistatic agent		olucto
buffer	catalyst	chelator		crosslinker	emollient	emulsifier	Cat	aiysts
stabilizer	film forming agent	flame retardant	flavorant)	foam boost. agent	foamer	fragrance		
conditioner	hair dye	stabilizer		lubricating agent	agent	monomer		slinkers
-I -I	pigment	oxidizer	[perfumer]	pH stabilizer	photoinitiator	plasticizer		
	reducer	rheology modifier	conditioner	skin protectant		solvent	Colo	orants
1.00 0.75 0.50 0.25 0.00		UV absorber		visc. control. agent	wetting agent	whitener		
Stand	lard Deviation lassification E	rror 🗔 5-	randomizatior fold Cross Val	n Error idation Error				





### Using the CompTox Dashboard to Get Data





### Searching by Chemical









SEPA Agency	Home Advanced Search Hexade 57-10-3   Searched by DS	Batch Search Lists V Canoic ac DTXSID2021 STox Substance Id.	bredictions cid 602	Downloads	Сору 🗸	Share -	Submit Comment	Q
DETAIL SEXECUTIVE SUMMARYPROPERTIESENV. FATE/TRANSPORTHAZARDHAZARDADMEEXPOSUREBIOACTIVITYSIMILAR COMPOUNDSGENRA (BETA)RELATED SUBSTANCESSYNONYMSLITERATURELINKSCOMMENTS	H <sub>3</sub> C			f	Wikipedi Palmitic ac nomenclatu fatty acid for microorgani CH3(CH2)14 name indica from the frui can also be dairy produce esters of pal  Read more Intrinsic Intrinsic Mol F Av and J Mol F Av g/mol Structura Record I	ia id, or hexadec re, is the most und in animals, sms. Its chemi COOH, and its its chemi tof oil palms (j found in meats cts. Palmitates lmitic acid. The Properties olecular Form file Q. Find verage Mass: 2 ope Mass Distri onoisotopic M al Identifier Substances e in Lists nformation	anoic acid in IUPAC common saturated plants and cal formula is C:D is 16:0. As its or component of the oi palm oil). Palmitic acid , cheeses, butter, and are the salts and palmitate ula: C10H32O2 All Chemicals 256.43 g/mol bution ass: 256.24023 S	



Separation United States Environmental Protection Agency	Home Advanced Search Batch Search Lists ∨ Predictions Downloads Hexadecanoic acid 57-10-3   DTXSID2021602 Searched by DSSTox Substance Id.	s Copy 👻 Share 👻 Submit Comment 📿
DETAIL S EXECUTIVE SUMMARY PROPERTIES ENV. FATE/TRANSPORT HAZARD ADME EXPOSURE BIOACTIVITY SIMILAR COMPOUNDS GENRA (BETA) RELATED SUBSTANCES SYNONYMS LITERATURE LINKS COMMENTS	$H_{3} \leftarrow H_{3} \leftarrow H_{3$	Wikipedia   Palmitic acid, or hexadecanoic acid in IUPAC nomenclature, is the most common saturated fatty acid found in animals, plants and microorganisms. Its chemical formula is CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> COOH, and its C:D is 16:0. As its name indicates, it is a major component of the oil from the fruit of oil palms (palm oil). Palmitic acid can also be found in meats, cheeses, butter, and dairy products. Palmitates are the salts and esters of palmitic acid. The palmitate   Image: Transition of the oil from the fruit of oil palms (palm oil). Palmitic acid can also be found in meats, cheeses, butter, and dairy products. Palmitates are the salts and esters of palmitic acid. The palmitate   Image: Transition of the oil from the fruit of oil palms (palm oil). Palmitic acid   Image: Transition of the oil from the fruit of oil palms (palm oil). Palmitic acid   Image: Transition of the oil from the fruit of oil palms (palm oil). Palmitic acid   Image: Transition of the oil from the fruit of oil palms (palm oil). Palmitic acid   Image: Transition of the oil from the fruit of oil palms (palm oil). Palmitic acid   Image: Transition of the oil from the fruit of oil palms (palm oil). Palmitic acid   Image: Transition of the oil from the fruit of oil palms (palm oil). Palmitic acid   Image: Transition of the oil from the fruit of oil from the fruit of oil palms (palm oil). Palmitic acid   Image: Transition of the oil from the fruit of oil from the fruit of oil palms (palm oil). Palmitates   Image: Transition of the oil from the fruit of oil from the f



	Agency	Hexadecapoic ac	Predictions Downloads Co	ypy ▼ Share ▼ Submit Comment Q S
		57-10-3   DTXSID2021 Searched by DSSTox Substance Id.	602	
	DETAILS	Product and	I Use Categories	(PUCs) 🚺
	EXECUTIVE SUMMARY	🛓 Download 👻		
	PROPERTIES	Columns ~ 10 V		Search query
	ENV. FATE/TRANSPORT	Product or Use Categorization	Categorization type	Number of Unique Products
	HAZARD		PUC	99
	▶ ADME	personal care: hand/body lotion	PUC	38
	✓ EXPOSURE	personal care: nail polish	PUC	30
	PRODUCT & USE CATEGORIES	personal care: shaving cream	PUC	17
	CHEMICAL WEIGHT FRACTION	personal care: mascara	PUC	12
		personal care: hair conditioner	PUC	11
	CHEMICAL FUNCTIONAL USE	personal care: shampoo	PUC	10
	TOXICS RELEASE INVENTORY	personal care: face cream/moisturizer	PUC	8
	MONITORING DATA	personal care: body wash	PUC	7
	EXPOSURE PREDICTIONS	lubricant	CPCat Cassette	7
	PRODUCTION VOLUME			
	BIOACTIVITY	First << < 1 2	3 4 5 6 7 8	9 10 > >> Last
	SIMILAR COMPOUNDS		Showing 1 to 10 of 105 records	
	GENRA (BETA)			
	RELATED SUBSTANCES			
	SYNONYMS			
fice of Research and Development	LITERATURE			



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	Hexadec	anoic a	acid				
	Searched by DSSTo	x Substance Id	21602				
DETAILS		Cher	nical We	ight Frac	tions 🚹		
EXECUTIVE SUMMARY	🛃 Download 👻						
PROPERTIES	Columns ~ 10 ~					Sear	ch query
ENV. FATE/TRANSPORT			Minimum	Maximum			
HAZARD	Product Name 🗘	Product Use Category \$	Weight Fraction \$	Weight Fraction \$	Data Type	\$	Source
▶ ADME	(diamond soap) for	personal care:	0.100	0.300	MSDS		Retail Product
	1	bui soup					Outegones/Walna
PRODUCT & USE CATEGORIES	air_freshener_1	-	2.42e-6	2.42e-6	EPA_SSA: tentative chemical class identification	÷	EPA Suspect Screening Research
CHEMICAL WEIGHT FRACTION	air_freshener_4	-	4.36e-6	4.36e-6	EPA_SSA: confirme	ed	EPA Suspect
CHEMICAL FUNCTIONAL USE					chemical identificat	IUT	Research
TOXICS RELEASE INVENTORY	aveeno positively	personal care: shaving cream			Ingredients List		DrugStore.com
MONITORING DATA	axe messy look paste	personal care:			Ingredients List		DruaStore.com
EXPOSURE PREDICTIONS	whatever 4	hair styling					
PRODUCTION VOLUME	baby_soap_2	-	5.30e-6	5.30e-6	EPA_SSA: confirme chemical identificat	ed ion	EPA Suspect Screening
BIOACTIVITY	hohy ocon 4		1 920 6	1 920 6	EBA SSA: confirm	ad.	EPA Support
SIMILAR COMPOUNDS	uduy_sudµ_4		1.028-0	1.028-0	chemical identificat	ion	Screening Research
GENRA (BETA)	baby_soap_5	-	2.31e-5	2.31e-5	EPA_SSA: confirme	ed	EPA Suspect
RELATED SUBSTANCES					chemical identificat	ion	Screening Research
SYNONYMS	barbasol aloe shave gel	personal care:			MSDS		Retail Product
	-	anaving creatil					Categories/wallia



United States Environmental Protection Agency	Home Advanced Search Batch Search Lists V Predictio	ns Downloads Copy - Share - Submit Comment
DETAILS	Collected Data	on Functional Use 🕦
EXECUTIVE SUMMARY	🛓 Download 👻	
PROPERTIES	Columns ~	Search query
ENV. FATE/TRANSPORT	Harmonized functional use	Reported functional use
HAZARD	fragrance	COLORANT
ADME	fragrance	EMOLLIENT
▼ EXPOSURE	-	emulsifier
PRODUCT & USE CATEGORIES	fragrance	EMULSIFYING
CHEMICAL WEIGHT FRACTION	fragrance	flavorant
CHEMICAL FUNCTIONAL USE	fragrance	fragrance
TOXICS RELEASE INVENTORY	fragrance	Lubricant
	- -	processing aid
		Surfactants
	_	
	_	
GENRA (BETA)	Predicted Probability of QSAR Versio	Associated Functional Use 1
RELATED SUBSTANCES		
SANONAMS		Coarch guogr
		Search query
LITERATURE	Harmonized functional use	Probability
	surfactant	0.934
LINKS		



SEPA United States Environmental Protection H Agency	ome Advanced Search Batch Search Lists 🗸 Predictions Downloads Copy 🔻 Share 💌 Submit Comment 🔍 Search
	Hexadecanoic acid
	57-10-3   DTXSID2021602
	Searched by DSSTox Substance Id.
DETAILS	National Health and Nutrition Examination Survey (NHANES)
EXECUTIVE SUMMARY	Inferences (mg/kg-bw/day)
PROPERTIES	There is no exposure monitoring data available.
ENV. FATE/TRANSPORT	
HAZARD	
▶ ADME	
EXPOSURE	Where's the data?!
PRODUCT & USE CATEGORIES	
CHEMICAL WEIGHT FRACTION	
CHEMICAL FUNCTIONAL USE	
TOXICS RELEASE INVENTORY	
MONITORING DATA	
EXPOSURE PREDICTIONS	
PRODUCTION VOLUME	
BIOACTIVITY	
SIMILAR COMPOUNDS	
GENRA (BETA)	



A

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SIMILAR COMPOUNDS

GENRA (BETA)

The Centers for Disease Control (CDC) National Health and Nutrition Examination Survey (NHANES) is a program of studies designed to assess the health and nutritional status of adults and children in the United States (link). As part of the NHANES, the CDC monitors biomarkers of chemical exposure (chiefly metabolites) in the blood and urine to quantify the levels of chemical compounds present in U.S. residents (link). Each two-year study cycle comprises approximately 10,000 individuals, with exposure biomarker data for any given chemical available from only a subset of roughly 1/3 of the individuals in the study. In the 2014 publication "High Throughput Heuristics for Prioritizing Human Exposure to Environmental Chemicals" (link) EPA scientists inferred steady state exposure rates (mg/kg bodyweight) for 106 chemicals from the NHANES urine samples. These 106 chemicals will have information below.

HANES)

#### There is only data for the 106 with inferred steady state exposure rates.



Agency	Diethyl phi 84-66-2   DTX Searched by DSSTox S	thalate SID7021780								
DETAILS	1 National H	ealth and Nutrit	ion Examinat	ion Survey (NHAN	IES)					
EXECUTIVE SUMMARY	Interences (mg/kg-bw/day)									
PROPERTIES	📥 Download 🔻									
ENV. FATE/TRANSPORT	Columns ~			Search query						
HAZARD	Demographic	Lower 95th Limit	Upper 950	th Limit	(					
	Ages 6-11	8.90e-4	1.10e-3	9.89e-4						
P ROME	Ages 12-19	8.22e-4	1.26e-3	1.02e-3						
▼ EXPOSURE	Ages 20-65	1.20e-3	1.52e-3	1.35e-3						
PRODUCT & USE CATEGORIES	Ages 65+	8.08e-4	1.21e-3	9.92e-4						
CHEMICAL WEIGHT FRACTION	BMI > 30	1.08e-3	1.32e-3	1.19e-3						
CHEMICAL FUNCTIONAL USE	BMI < 30	1.17e-3	1.31e-3	1.24e-3						
TOXICS RELEASE INVENTORY	Repro. Age Females	1.32e-3	1.62e-3	1.46e-3						
	Females	1.16e-3	1.44e-3	1.30e-3						
MONITORING DATA	Males		1.30e-3	1.15e-3						
EXPOSURE PREDICTIONS	Total	1.16e-3	1.29e-3	1.22e-3						
PRODUCTION VOLUME										
▶ BIOACTIVITY			10 records							
SIMILAR COMPOUNDS										



EF	United States Environmental Protection Agency	Home Advanced Search	Batch Search Lists 🗸	Predictions Downloa	ads Copy	▼ Share ▼	Submit Comment	Q Sea
		Hexade 57-10-3   [ Searched by Appr	Canoic ac DTXSID2021 roved Name.	602				
	DETAILS		🚺 Expos	ure Predicti	<b>ons</b> <u>(m</u>	g/kg-bw/day	)	
	EXECUTIVE SUMMARY	📩 Download 🔻						
	PROPERTIES	Columns ~					Search query	
	ENV. FATE/TRANSPORT	Demographic		Median	\$	95th Percentile		\$
	HAZARD	Ages 6-11		1.17e-4		1.03e-2		
Þ	ADME	Ages 12-19		8.76e-5		4.04e-3		
-	EXPOSURE	Ages 20-65		8.89e-5		5.39e-3		
		Ages 65+		5.26e-5		2.99e-3		
	PRODUCT & USE CALEGORIES	BMI > 30		6.32e-5		5.82e-3		
	CHEMICAL WEIGHT FRACTION	BMI < 30		9.56e-5		4.55e-3		
	CHEMICAL FUNCTIONAL USE	Repro. Age Females		1.03e-4		6.61e-3		
	TOXICS RELEASE INVENTORY	Females		7.93e-5		5.88e-3		
		Males		8.96e-5		4.51e-3		
	MONITORING DATA	Total		7.89e-5		5.73e-3		
	EXPOSURE PREDICTIONS							
	PRODUCTION VOLUME			10 records				
Þ	BIOACTIVITY							
	SIMILAR COMPOUNDS							
	GENRA (BETA)							
pa.gov								



E	United States Environmental Protection Agency	Home Advanced Search Batch	ı Search Lists ✔ Pre	dictions Downloads C	opy 🔻 Share 🔻	Submit Comment	<b>λ</b> s
		Hexadeca 57-10-3   DT> Searched by Approved	noic acid (SID202160 <sub>Name.</sub>	2			
	DETAILS	_	f Exposure	Predictions	mg/kg-bw/day	<u>)</u>	
	EXECUTIVE SUMMARY	🛓 Download 👻	-				
	PROPERTIES	Columns ~				Search query	
	ENV. FATE/TRANSPORT	Demographic	÷	Median	<u>95th Percentile</u>		\$
	HAZARD	Ages 6-11		1.17e-4	1.03e-2		
•	ADME	Ages 12-19		8.76e-5	4.04e-3		
	EXPOSURE	Ages 20-65		8.89e-5	5.39e-3		
		Ages 65+		5.26e-5	2.99e-3		
		BMI > 30		6.32e-5	5.82e-3		
	CHEMICAL WEIGHT FRACTION	BMI < 30		9.56e-5	4.55e-3		
	CHEMICAL FUNCTIONAL USE	Repro. Age Females		1.03e-4	6.61e-3		
	TOXICS RELEASE INVENTORY	Females		7.93e-5	5.88e-3		
	MONITORING DATA	Males		8.96e-5	4.51e-3		
		Total		7.89e-5	5.73e-3		
	PRODUCTION VOLUME			10 records			
	BIOACTIVITY						
	SIMILAR COMPOUNDS						
	GENRA (BETA)						



### Searching by Product and Use Categories





SEPA United States Environmental Prot Agency	ection Home Advance	d Search Batch Search Lists 🗸	Predictions Downloads		Share 🔻		
WITED STATES		762 Thousa	nd Chemicals				
	Chemicals Product/Use Categories Assay/Gene						
AGE							
WTAL PROTECTIO	CPDat PRODUCT category: personal care hair color hair colors and dyes characterized as permanent						
	CPDat PRODUCT category: personal care hair color hair colors and dyes characterized as for professional use CPDat PRODUCT category: personal care hair color hair colors and dyes characterized as temporary						
	CPDat PRODUCT category: personal care hair color hair coloring products not otherwise categorized						
	CPDat PRODUCT category: personal care hair color activator chemical activators for hair coloring products						
	CPDat PRODUCT category: personal care hair color developer chemical developers for hair coloring products						
•	CPDat PRODUCT category: personal care hair color toner chemical toners for hair coloring products						
	CPDat PRODUCT category: personal care lip color colored lip products, excluding glosses						
	CPCat USE category: colorant term used for colorants, dyes, or pigments; includes colorants for drugs, textiles, personal care products (cosmetics, tatoo inks, hair dye), food colorants, and inks for printing; modifier						
	CPCat USE category: colorant_ACToRUseDB specific term assigned only to sources from the ACToR UseDB related to colorants or dyes (note the **_ACToRUseDB" terms are assigned to more general groups and thus may not						
	ED STATE	Discover	Connect	Ask			
- ENVIRG	<b>Bend</b>	About/Disclaimer	ACTOR	Contact			
And the second se	L PROTECTION	Accessibility Privacy	DSS fox Downloads	нер			



EPA Environmenta	I Protection Home Advanced Search Bate	ch Search Lists ✔ Predictions Downloads				Share 🔻 🔍 Searc	ch all data
			Searched by Produ Results for CPCat Use Cat	egory: CPCat term: Colorant			
			2167 cl	hemicals			
Download / Send 👻					Show info:	DTXSID × CASRN × TOXCAST	💌 👻 Select all
rt by: DTXSID 👻 î						Filter by: Name or CASRN	Hide -
	0 related chemical	0 related chemical	0 related chemical	0 related chemical	0 related chemical	0 related chemical	
	structures with this	structures with this	structures with this	structures with this	structures with this	structures with this	
	substance	substance	substance	substance	substance	substance	
	Iron manganese oxide ((Fe,Mn)2O3) DTXSID: DTXSID00104976	1-Naphthalenesulfonic acid, 5-hydroxy-, DTXSID: DTXSID00105105	Lignin, alkali, reaction products with dis DTXSID: DTXSID00105862	Octadecanoic acid, 12-hydroxy-, homop DTXSID: DTXSID00106172	Naphthalenesulfonic acid, methyl-, poly DTXSID: DTXSID00108419	C.I. Direct Blue 42 DTXSID: DTXSID00108772	
	CASRN: 75864-23-2 TOXCAST: 0	CASRN: 79873-34-0 TOXCAST: 0	CASRN: 105859-97-0 TOXCAST: 0	CASRN: 124578-12-7 TOXCAST: 0	CASRN: 81065-51-2 TOXCAST: 0	CASRN: 6426-71-7 TOXCAST: 0	
	0 related chemical	0 related chemical	H <sub>3</sub> C	H <sub>2</sub> N	ОН	^	
	structures with this	structures with this			o o		
	substance	substance	CI NH2	H₃C∽ СІ			
	O L Direct Down 10	Debuters 4.0 effects (5.0) white bildress	0 Oblass 4 staffindes/line	nei	2.4 Distantianal	Ethology guide	
	C.I. DIrect Brown 13 DTXSID: DTXSID00108777 CASEN: 8003-82-5	DTXSID: DTXSID00110077	DTXSID: DTXSID020286	4-Chioro-2-methylaniline hydrochionde DTXSID: DTXSID0020288 CASDN: 3165-93-3	DTXSID: DTXSID0020523	DTXSID: DTXSID0020600	
	TOXCAST: 0	TOXCAST: 0	TOXCAST: 5/297	TOXCAST: 9/276	TOXCAST: 32/508	TOXCAST: 0	
	2+						_
	CI CI		N	NH <sub>2</sub>		1 related chemical	
	њо њо њо	CI CI	0 0			structure with this	
	но но но		Na	₀″ \/ \сн₃	nin – upř	substance	
	Magnesium chloride hexabydrate	Dichloromethane	Sodium pitrite	2-Methoxy-5-nitroaniline	4.4'-Oxydianiline	Polysorbate 80	
	DTXSID: DTXSID0020789 CASRN: 7791-18-6	DTXSID: DTXSID0020868 CASRN: 75-09-2	DTXSID: DTXSID0020941 CASRN: 7632-00-0	DTXSID: DTXSID0020943 CASRN: 99-59-2	DTXSID: DTXSID0021094 CASRN: 101-80-4	DTXSID: DTXSID0021175 CASRN: 9005-65-6	
	TOXCAST: 3/113	TOXCAST: 1/113	TOXCAST: 3/537	TOXCAST: 14/572	TOXCAST: 29/589	TOXCAST: 10/297	



Sepa United States Environmental Agency	Protection Home Advanced Search Batch	Search Lists   Predictions Downloads				Share 🔻 🔍 Searc	ch all data
			Searched by Produce Results for CPCat Use Cate	t & Use Categories			
			2167 che	micals			
Download / Send 👻					Show info:	DTXSID × CASRN × TOXCAST	💌 👻 Select all
iort by: DTXSID 🔻 î						Filter by: Name or CASRN	Hide -
				•	P		)
	0 related chemical	0 related chemical	0 related chemical	0 related chemical	0 related chemical	0 related chemical	
	structures with this	structures with this	structures with this	structures with this	structures with this	structures with this	
	substance	substance	substance	substance	substance	substance	
	Iron manganese oxide ((Fe,Mn)2O3)	1-Naphthalenesulfonic acid, 5-hydroxy	Lignin, alkali, reaction products with dis	Octadecanoic acid, 12-hydroxy-, homop	Naphthalenesulfonic acid, methyl-, poly	C.I. Direct Blue 42	
	DTXSID: DTXSID00104976 CASRN: 75864-23-2	DTXSID: DTXSID00105105 CASRN: 79873-34-0	DTXSID: DTXSID00105862 CASRN: 105859-97-0	DTXSID: DTXSID00106172 CASRN: 124578-12-7	DTXSID: DTXSID00108419 CASRN: 81065-51-2	DTXSID: DTXSID00108772 CASRN: 6426-71-7	
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	substance	substance	CI NH2	H <sub>3</sub> C CI			
				нсі			
	C.I. Direct Brown 13 DTXSID: DTXSID00108777 CASRN: 8003.82-5	Poly(oxy-1,2-ethanediyi), alpha-tridecyl DTXSID: DTXSID00110077 CASRN: 69011.36.5	3-Chloro-4-methylaniline DTXSID: DTXSID0020286 CASRN: 95-74-9	4-Chloro-2-methylaniline hydrochlonde DTXSID: DTXSID0020288 CASRN: 3165-93-3	2,4-Dinitrophenol DTXSID: DTXSID0020523 CASRN: 51-28-5	DTXSID: DTXSID0020600	
	TOXCAST: 0	TOXCAST: 0	TOXCAST: 5/297	TOXCAST: 9/276	TOXCAST: 32/508	TOXCAST: 0	
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	2+ Mg		N				
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	H <sub>2</sub> O H <sub>2</sub> O H <sub>2</sub> O	CI CI			Here I have a second se	structure with this	
	H <sub>2</sub> O H <sub>2</sub> O H <sub>2</sub> O		Nđ	• — eng		Substance	
	Magnesium chloride hexahydrate DTXSID: DTXSID0020789	Dichloromethane DTXSID: DTXSID0020868	Sodium nitrite DTXSID: DTXSID0020941	2-Methoxy-5-nitroaniline DTXSID: DTXSID0020943	4,4'-Oxydianiline DTXSID: DTXSID0021094	Polysorbate 80 DTXSID: DTXSID0021175	
	CASRN: 7791-18-6 TOXCAST: 3/113	CASRN: 75-09-2 TOXCAST: 1/113	CASRN: 7632-00-0 TOXCAST: 3/537	CASRN: 99-59-2 TOXCAST: 14/572	CASRN: 101-80-4 TOXCAST: 29/589	CASRN: 9005-65-6 TOXCAST: 10/297	









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