

- **ToxTool<sup>®</sup> : online toxicological database**

- A new competitiveness tool for the Safety Assessors and R&D teams of every cosmetic company

**Dr. Matteo Zanotti Russo**



## Safety Assessment

- ▶ Scientific act
- ▶ Multifactorial
- ▶ Thoughtful

## Expert Judgment

## DATA

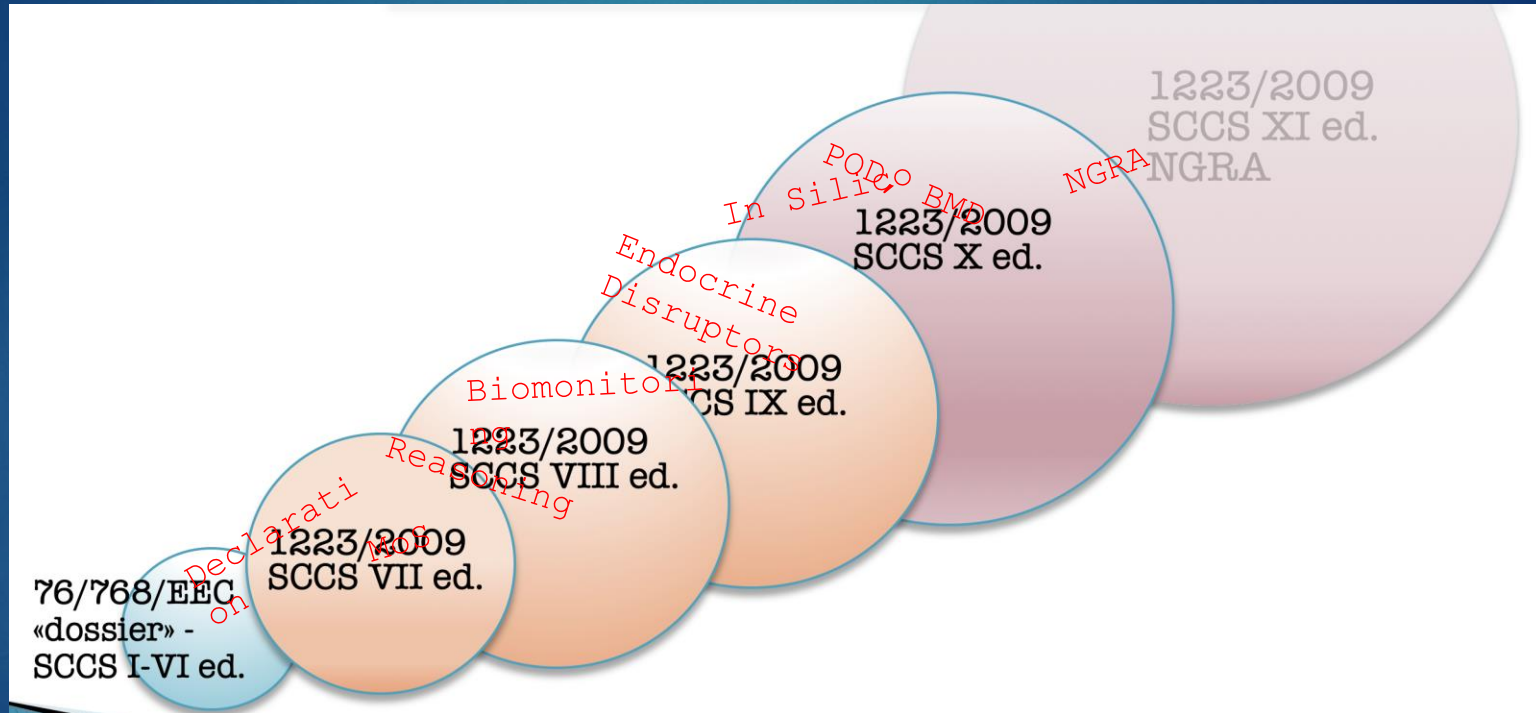


CPSR-A



CPSR-B

## SCCS NoG: Evolution



## Data source

- ▶ Numerous sources of information:
  - ▶ Supplier
  - ▶ CIR, SCCS, ECHA
  - ▶ Scientific literature
  - ▶ Patent Literature
  - ▶ In silico
- Thousands of pages to extrapolate from:
  - toxicological data
  - Evidence (comments)
- The data form the basis for the evaluation of the finished cosmetic
- ▶ PIF/SA Updated! (Reg. 1223/2009 art 10.1 c)

→ **DATABASE!**



## Database

- ▶ Uses:
  - ▶ Exposure table and MoS calculation
  - ▶ Global view of the salient elements
  - ▶ The Evaluator has an overall "overview" essential for drafting the CPSR-B (evaluation and reasoning)
  - ▶ Identification of parameters (impurities) and criticalities



- **representative and user driven:** the most used ingredients are already present in the database, but the ingredients not yet present can be requested at no additional cost

- **proprietary data and reasoning:** implemented with the latest in silico methodologies, processed by qualified experts on European platforms validated by ECHA and SCCS. A reasoning for each ingredient, so as to better support the evaluation of the finished product

**updated:** Toxicological data and frames always updated. NGRA ready...

- **user friendly:** intuitive and immediate use without courses, local installations, updates, user manuals. It is accessed from the web with LogonID and Password

- **shared:** the database is consulted and shared among a growing number of Safety Assessors. The documents created to help you in the creation of PIF and CPSR will carry a ToxTool® security QR code

- **protected:** the data is kept on a proprietary server. The documents created bear a ToxTool® security QR code which associates the document with the company.

## Fundamental for

- the regulatory team of each cosmetic company
- the Security Evaluator
- the R&D team, according to the most current Safe by Design approaches



# ToxTool

The innovative easy-to-use platform for *cosmetics* safety assessment

ToxTool®: online toxicological database



- **Structured:** Created and continuously implemented by a team of qualified Safety Assessors and independent academics

- **Endorsed:** Scientific Supervision of the University of Genoa, Department of Earth, Environment and Life Sciences - Team of Prof. Elena Grasselli.

- **Powered by:**



## Fundamental for

- the regulatory team of each cosmetic company
- the Security Evaluator
- the R&D team, according to the most current Safe by Design approaches





UDRD-User Driven Reasoned Database

# The innovative easy-to-use IT platform for cosmetic safety assessments

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# ToxTool

The innovative easy-to-use platform for *cosmetics* safety assessment

# ToxTool

Landing Page

ToxTool®: online toxicological database



Login to your account

Username required

Password required

Remember me

[Forgot password?](#)



3948 records, showing 0-17

Basic info | Substance reasoning | Regulatory status and scientific literature | Substance Information | Toxicological Data

Id	INCI	CAS	EINECS	Cosmetic function	Date modified
5929	MENTHYL ETHYLAMIDO OXALATE	1122460-01-8		skin conditioning	2022-07-13 12:22
5928	MENTHA VIRIDIS (SPEARMINT) EXTRACT	84696-51-5 / 90064-01-0	283-656-2	fragrance, oral care	2022-07-13 12:22
4264	MELALEUCA ALTERNIFOLIA OIL	85085-48-9 / 8022-72-8 / 68647-73-4	285-377-1 / - / -	Antioxidant, Perfuming	2022-07-13 12:22
4263	MELALEUCA ALTERNIFOLIA (TEA TREE) OIL	85085-48-9 / 8022-72-8 / 68647-73-4	285-377-1 / - / -	Antioxidant, Perfuming	2022-07-13 12:22
4262	MELALEUCA ALTERNIFOLIA (TEA TREE) LE...	85085-48-9 / 8022-72-8 / 68647-73-4	285-377-1 / - / -	Antioxidant, Perfuming	2022-07-13 12:00
4176	LYCIUM BARBARUM FRUIT EXTRACT	85085-46-7	285-375-0	Astringent, Hair conditioning, Skin conditioning	2022-07-13 11:59
4175	LYCIUM BARBARUM (MATRIMONY VINE) F...	85085-46-7	285-375-0	Astringent, Hair conditioning, Skin conditioning	2022-07-13 11:54
4155	LINUM USITATISSIMUM (LINSEED) SEED OIL	8001-26-1	232-278-6	Perfuming, skin conditioning	2022-07-13 11:11
4111	LAURYL PEG-9 POLYDIMETHYLSILOXYETH...	-	-	Hair conditioning, Skin conditioning, Surfactant, emulsifier	2022-07-13 11:15
4069	LACTOSE	63-42-3	200-559-2	Humectant, skin conditioning	2022-07-13 11:00
5927	HYSSOPUS OFFICINALIS EXTRACT	84603-66-7	283-266-2	fragrance, tonic	2022-07-13 11:00
3894	HYDROLYZED RICE PROTEIN	156715-40-1	-	Antistatic, hair conditioning, skin conditioning	2022-07-13 10:30
3889	HYDROLYZED PEA PROTEIN	222400-29-5	-	antistatic, emollient, hair conditioning, hair conditioning, skin conditioning	2022-07-13 10:20

3948 records, showing 0-17

Basic info

**Substance reasoning**

Regulatory status and scientific literature

Substance Information

Toxicological Data

Id	INCI		Safety Assessment
5929	MENTHYL ETHYLAMIDO OXALATE		Menthyl Ethylamido Oxalate is a organic compound. According to information available on ECHA website this substance can be considered irritating for human skin ...
5928	MENTHA VIRIDIS (SPEARMINT) EXTRACT		Mentha Viridis Extract is an extract of the whole plant of the Garden Mint (spearmint), Mentha viridis L., Labiatae
4264	MELALEUCA ALTERNIFOLIA OIL		Melaleuca Alternifolia Leaf Oil is the oil distilled from the leaves of the Tea Tree, Melaleuca alternifolia, Myrtaceae . Tea Tree Oil is a skin sensitiser. Skin sensitisation m...
4263	MELALEUCA ALTERNIFOLIA (TEA TREE) OIL		Melaleuca Alternifolia Leaf Oil is the oil distilled from the leaves of the Tea Tree, Melaleuca alternifolia, Myrtaceae . Tea Tree Oil is a skin sensitiser. Skin sensitisation m...
4262	MELALEUCA ALTERNIFOLIA (TEA TREE) LE...		Melaleuca Alternifolia Leaf Oil is the oil distilled from the leaves of the Tea Tree, Melaleuca alternifolia, Myrtaceae . Tea Tree Oil is a skin sensitiser. Skin sensitisation m...
4176	LYCIUM BARBARUM FRUIT EXTRACT		The berries of Lycium barbarum, a perennial plant native to Asia and southeastern Europe, have been used for centuries in traditional Chinese medicine. They are als...
4175	LYCIUM BARBARUM (MATRIMONY VINE) F...		The berries of Lycium barbarum, a perennial plant native to Asia and southeastern Europe, have been used for centuries in traditional Chinese medicine. They are als...
4155	LINUM USITATISSIMUM (LINSEED) SEED OIL		Linum Usitatissimum Seed Oil is the expressed oil from the dried ripe seed of the Linseed, Linum usitatissimum L., Linaceae. This fatty oil is edible, and exposure to th...
4111	LAURYL PEG-9 POLYDIMETHYLSILOXYETH...		Lauryl PEG-9 polydimethylsiloxyethyl dimethicone is the silicone polymer that can be described as siloxanes and silicones, dodecyl methyl, 2-trimethylsilyloxydi...
4069	LACTOSE		Lactose is a sugar which occurs in mammals milk, chemically it can be defined as disaccharide of glucose and galactose. It is used as a nutrient and can used also as...
5927	HYSSOPUS OFFICINALIS EXTRACT		Hyssopus Officinalis Extract is an extract of the leaves of the Hyssop, Hyssopus officinalis L., Labiatae
3894	HYDROLYZED RICE PROTEIN		Hydrolyzed Rice Protein is a hydrolysate of rice protein derived by acid, enzyme or other method of hydrolysis. Rice is the seed of the grass species Oryza sativa, a cer...
3889	HYDROLYZED PEA PROTEIN		Hydrolyzed Pea Protein is the hydrolysate of pea protein derived by acid, enzyme or other method of hydrolysis. Hydrolyzed Pea Protein it is not skin irritating. It is lar...
5926	HYDROLYZED HEMP SEED EXTRACT		Hydrolyzed Hemp Seed Extract is the hydrolysate of an extract of Cannabis Sativa Seed derved by acid, enzyme or other method of hydrolysis.

3948 records, showing 0-17

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Substance reasoning

Regulatory status and scientific literature

Substance Information

Toxicological Data

Id	INCI		Safety Assessment
5929	MENTHYL ETHYLAMIDO OXALATE		Menthyl Ethylamido Oxalate is an organic compound. According to information available on ECHA website this substance can be considered irritating for human skin ...
5928	MENTHA VIRIDIS (SPEARMINT) EXTRACT		Mentha Viridis Extract is an extract of the whole plant of the Garden Mint (spearmint), Mentha viridis L., Labiatae
4264	MELALEUCA ALTERNIFOLIA OIL		Melaleuca Alternifolia Leaf Oil is the oil distilled from the leaves of the Tea Tree, Melaleuca alternifolia, Myrtaceae. Tea Tree Oil is a skin sensitiser. Skin sensitisation m...
4263	MELALEUCA ALTERNIFOLIA (TEA TREE) OIL		Melaleuca Alternifolia Leaf Oil is the oil distilled from the leaves of the Tea Tree, Melaleuca alternifolia, Myrtaceae. Tea Tree Oil is a skin sensitiser. Skin sensitisation m...
4262	MELALEUCA ALTERNIFOLIA (TEA TREE) LE...		Melaleuca Alternifolia Leaf Oil is the oil distilled from the leaves of the Tea Tree, Melaleuca alternifolia, Myrtaceae. Tea Tree Oil is a skin sensitiser. Skin sensitisation m...
4176	LYCIUM BARBARUM FRUIT EXTRACT		The berries of Lycium barbarum, a perennial plant native to Asia, have been used for centuries in traditional Chinese medicine. They are als...
4175	LYCIUM BARBARUM (MATRIMONY VINE) F...		The berries of Lycium barbarum, a perennial plant native to Asia, have been used for centuries in traditional Chinese medicine. They are als...
4155	LINUM USITATISSIMUM (LINSEED) SEED OIL		Linum Usitatissimum Seed Oil is the expressed oil from the dried seeds of the flax plant, Linum usitatissimum L., Linaceae. This fatty oil is edible, and exposure to th...
4111	LAURYL PEG-9 POLYDIMETHYLSILOXYETH...		Lauryl PEG-9 polydimethylsiloxethyl dimethicone is the silicone oil distilled from the leaves of the Tea Tree, Melaleuca alternifolia, Myrtaceae. Tea Tree Oil is a skin sensitiser. Skin sensitisation may also be enhanced by irritancy, Tea Tree Oil and certain formulations at concentrations of 5% or more can induce skin and eye irritation. The safe use of Tea Tree Oil as cosmetic ingredient cannot be assessed, so SCCP suggests to use this ingredient up to 1%. According to ECHA website the dermal absorption is 3%
4069	LACTOSE		Lactose is a sugar which occurs in mammals milk, chemically it is a disaccharide composed of glucose and galactose. It is used as a nutrient and can used also as...
5927	HYSSOPUS OFFICINALIS EXTRACT		Hyssopus Officinalis Extract is an extract of the leaves of the Hyssopus officinalis L., Lamiaceae.
3894	HYDROLYZED RICE PROTEIN		Hydrolyzed Rice Protein is a hydrolysate of rice protein derived by acid, enzyme or other method of hydrolysis. Rice is the seed of the grass species Oryza sativa, a cer...
3889	HYDROLYZED PEA PROTEIN		Hydrolyzed Pea Protein is the hydrolysate of pea protein derived by acid, enzyme or other method of hydrolysis. Hydrolyzed Pea Protein it is not skin irritating. It is lar...
5926	HYDROLYZED HEMP SEED EXTRACT		Hydrolyzed Hemp Seed Extract is the hydrolysate of an extract of Cannabis Sativa Seed derived by acid, enzyme or other method of hydrolysis.



Melaleuca Alternifolia Leaf Oil is the oil distilled from the leaves of the Tea Tree, Melaleuca alternifolia, Myrtaceae. Tea Tree Oil is a skin sensitiser. Skin sensitisation may also be enhanced by irritancy, Tea Tree Oil and certain formulations at concentrations of 5% or more can induce skin and eye irritation. The safe use of Tea Tree Oil as cosmetic ingredient cannot be assessed, so SCCP suggests to use this ingredient up to 1%. According to ECHA website the dermal absorption is 3%

3948 records, showing 0-17

Basic info   Substance reasoning   **Regulatory status and scientific literature**   Substance Information   Toxicological Data

Id	INCI	EU Reg 1223/2009 Annexes	Harmonised CLP classification	Scientific Literature
5929	MENTHYL ETHYLAMIDO OXALATE			ECHA website Brief Profile - Last updated: 21/03/2022
5928	MENTHA VIRIDIS (SPEARMINT) EXTRACT			
4264	MELALEUCA ALTERNIFOLIA OIL			* SCCS/0843/04 - Opinion on Tea Tree Oil * SCCS/11...
4263	MELALEUCA ALTERNIFOLIA (TEA TREE) OIL			\- SCCS/0843/04 - Opinion on Tea Tree Oil \- SCCS/1...
4262	MELALEUCA ALTERNIFOLIA (TEA TREE) LE...			\- SCCS/0843/04 - Opinion on Tea Tree Oil \- SCCS/1...
4176	LYCIUM BARBARUM FRUIT EXTRACT			
4175	LYCIUM BARBARUM (MATRIMONY VINE) F...			
4155	LINUM USITATISSIMUM (LINSEED) SEED OIL			* CIR Final Report on Plant-Derived Fatty Acid Oils a...
4111	LAURYL PEG-9 POLYDIMETHYLSILOXYETH...			CIR - Safety Assessment of Polyoxyalkylene Siloxane...
4069	LACTOSE			* CIR - Safety Assessment of Monosaccharides, Disa...
5927	HYSSOPUS OFFICINALIS EXTRACT			* CIR - Safety Assessment of Monosaccharides, Disaccharides, and Related Ingredients as Used in
3894	HYDROLYZED RICE PROTEIN			IJT 25(S
3889	HYDROLYZED PEA PROTEIN			CIR Saf
5926	HYDROLYZED HEMP SEED EXTRACT			EMA/CHMP/186428/2016 * IJT Cosmetics, April 4, 2014 - EMA/CHMP/186428/2016 * IJT 38(Suppl. 1):5-38, 2019 * EMA/CHMP/186428/2016



3948 records, showing 78-98

Basic info

Substance reasoning

Regulatory status and scientific literature

Substance Information

Toxicological Data

Id	INCI	MW	Log K <sub>ow</sub> (Octanol-Water)	Melting point	Boiling point
2505	BASIC BLUE 124	305.8 g/mol	-1.79 (pH 6.2, 23°C); 1-Octanol/water (shak...	>225 °C (OECD 102)	
5899	DIMETHYLAMINOPROPYLAMINE (DMAPA)				
5898	AMIDOAMINE (AA)	-	-	-	-
2046	DIMETHICONE	236.534 g/mol		-35°C	155-220°C
2102	STEARIC ACID	284.484 g/mol	Log Pow 8.23	63.89 - 71.2 °C	232 - 385.8 °C @ 19.998 - 1
2056	GLYCERYL STEARATE	358.57 g/mol	5.63 - 15.07	66.7 °C	
2008	CETEARYL ALCOHOL	512.9 g/mol	6.73 @ 25 °C and pH 7	57.74 °C	330.79 °C
2054	GLYCERIN	92.09382 g/mol	-1.75 @ 25 °C and pH 7.4	18.17 °C @ 101.3 kPa	290 °C @ 101.325 kPa
3574	FORMALDEHYDE	30.026 g/mol	ECHA: 0.35 @ 25 °C	ECHA: -118.3 - -9 °C @ 101.3 - 101.325 kPa	ECHA: -21 - 101 °C @ 101.3
5895	ETHYLENE OXIDE	44.053 g/mol	ECHA: -0.3 @ 25 °C	ECHA: -111.7 °C	ECHA: 10.7 °C
1988	ALOE BARBADENSIS LEAF JUICE		-2.58 @ 20 °C and pH 7		
2039	COCAMIDOPROPYL BETAINE	342.5 g/mol	-1.28	0 °C	104.3 °C
2101	SODIUM LAURETH SULFATE	Sodium 2-(2-dodecyloxyethoxy)ethyl sulph...	Sodium 2-(2-dodecyloxyethoxy)ethyl sulph...	2-dodecoxyethyl hydrogen sulfate- 150 - 3...	Sodium 2-(2-dodecyloxyetho
2427	AQUA (WATER)	18.015 g/mol	-	0 °C	100°C

Do you need more information?

*Molecular Weight, Log KOW (Octanol-Water), Melting point, Boiling point, Water solubility, Other physical/chemical data, Bioavailability summary, Dermal absorption, Oral bioavailability, Inhalatory bioavailability*

3948 records, showing 78-98


		Basic info	Substance reasoning	Regulatory status and scientific literature	Substance Information	Toxicological Data
Id	INCI	Skin irritation	Eye irritation	Skin sensitization	Photo-induced toxicity	
2508	BASIC BROWN 17	SCCS/1531/14: In dermal irritation studies...	SCCS/1531/14: Basic Brown 17 was predic...	SCCS/1531/14: Basic Brown 17 (purity > 94...		
2506	BASIC BLUE 99	ECHA: No adverse effect observed (not irr...	ECHA: No adverse effect observed (not irrit...	ECHA: Adverse effect observed (sensitising...		
2505	BASIC BLUE 124	SCCS/1542/14: In a dermal irritation stud...	SCCS/1542/14: In an eye-irritation study in ...	SCCS/1542/14: Two LLNA tests in mice and...		
5899	DIMETHYLAMINOPROPYLAMINE (DMAPA)	-	-	skin sensitiser	-	
5898	AMIDOAMINE (AA)	-	-	skin sensitiser	-	
2046	DIMETHICONE	CIR: Skin irritation was tested by gently ru...	CIR: Sixteen adult pigmented rabbits were t...	CIR: In a human repeat insult patch test (H...		
2102	STEARIC ACID	CIR: Skin irritation was tested by gently rubbing 0.5 mL of Dimethicone (100 cm2/sec) daily on a 2.5 cm 2 closely shaven skin patch of 3 rabbits and 3 guinea pigs for 10 days, which were then observed for 15 days. No erythema or signs of skin irritation or inflammation was noted in the animals.	not irritating	not sensitising	Cosmetic product formulation	
2056	GLYCERYL STEARATE	CIR: In primary eye irritation studies, glyceryl ste...	In primary eye irritation studies, glyceryl ste...	Glyceryl stearate at concentrations of up to ...	Glyceryl stearate at concentr	
2008	CETEARYL ALCOHOL	A...	Additionally, the classification provided by c...	No evidence of sensitization was produced.		
2054	GLYCERIN	CIR: Non-Human Glycerin was not irritating...	CIR: Non-Human Glycerin was not irritating...	CIR: Non-HumanNatural and synthetic glyc...		
3574	FORMALDEHYDE	ECHA: Adverse effect observed (corrosive)	ECHA: Adverse effect observed (irritating)	ECHA: Adverse effect observed (sensitising)		
5895	ETHYLENE OXIDE	ECHA: Adverse effect observed (corrosive)	ECHA: Adverse effect observed (irreversible...	ECHA: No adverse effect observed (not sen...		
1988	ALOE BARBADENSIS LEAF JUICE	The classification provided by companies ...	The classification provided by companies to...	-	-	
2039	COCAMIDOPROPYL BETAINE	CIR: In rabbits, CAPB was not considered ...	The classification provided by companies to...	A majority of data submitters agree this su...	CIR: n investigation of the po	

### Do you need Toxicological data?

*Skin irritation, Eye irritation, Skin sensitization, Photo-induced toxicity, Dermal sensitization, Repeated toxicity data, Acute toxicity data, Toxicity to reproduction data, Genetic toxicity / Carcinogenicity data, Endocrine activity (NGRA), Organospecific toxicity (NGRA), TTC, Selected POD*







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174 records, showing 0-17

Basic info
Substance reasoning
Regulatory status and scientific literature
Substance Information
Toxicological Data

Id	INCI	CAS	EINECS	Cosmetic function	Date modified ↓
4111	LAURYL PEG-9 POLYDI-METHYLSILOXYET...	-	-	Hair conditioning, Skin conditioning, Surfactant, emulsifier	2022-07-13 11:12
5913	CITRONELLYL METHYLCROTONATE	20770-40-5	244-019-4	Fragrance, Perfuming	2022-07-12 09:46
5899	DI-METHYLAMINOPROPYLAMINE (DMAPA)	-	-	technically unavoidable impurity	2022-06-29 19:06
2371	AMINO-METHYL PROPANOL	124-68-5	204-709-8	Buffering	2022-06-21 10:08
2370	AMINO-METHYL PROPANEDIOL	115-69-5	204-100-7	Buffering	2022-06-21 09:30
1990	ALPHA-ISO-METHYL IONONE	127-51-5	204-846-3	Perfuming, Skin Conditioning	2022-06-17 11:02
2330	ALLYL TRIMETHYLHEXANOATE	68132-80-9	268-648-9	perfuming	2022-06-16 15:18
2314	ALLYL 3,5,5-TRIMETHYLHEXANOATE	71500-37-3	275-536-3	Perfuming	2022-06-13 09:19
2313	ALLYL 2-METHYLBUTOXYACETATE	67634-01-9	266-804-0	perfuming	2022-06-13 09:11
2218	ACETYL HEXAMETHYL TETRALIN	1506-02-1 / 21145-77-7	216-133-4 / 244-240-6	Masking	2022-06-08 13:00
2217	ACETYL HEXAMETHYL INDAN	15323-35-0	239-360-0	Masking, Perfuming, Fragrance	2022-06-08 12:54
2172	6-METHOXY-2-METHYLAMINO-3-AMINOP...	90817-34-8 / 83732-72-3	- / 280-622-9	Hair Dyeing	2022-06-07 09:40
2165	4-METHYLBENZYLIDENE CAMPHOR	36861-47-9 / 38102-62-4	253-242-6 /	UV absorber, UV filter	2022-06-06 10:47
2156	3-METHYLNON-2-ENENITRILE	53153-66-5	258-398-9	Perfuming	2022-06-01 16:51

Looking for ingredients



**BENZOIC ACID**  
CAS: 65-85-0

Cosmetic function  
Fragrance Preservative pH Adjusters

EINECS  
200-618-2

SMILES  
OC(=O)C1=CC=CC=C1

Impurities  
-

marco.pirozzi
 

Created  
03/07/2021 00:00

Last modified  
01/01/2022 12:00

Overview
Substance Information
Toxicity
Attached Documentation (1)
Versions (2)

**Substance identity**

INCI BENZOIC ACID	CAS 65-85-0
EINECS 200-618-2	SMILES <chem>OC(=O)C1=CC=CC=C1</chem>

**Summary / Substance reasoning**

Benzoic acid is an aromatic acid. Largely used as food supplement it is generally recognized as safe. SCCP is of the opinion that Benzoic acid is safe for use for preservative and non-preservative purposes in cosmetic rinse-off products at a maximum concentration of 2.5 % and in cosmetic oral-care products at a maximum concentration of 1.7 %, and in leave-on products up to 0.5%.

**Regulatory status**

**Reg 1223/2009 Annexes**  
Annex V/1 Product Type, body parts a) Rinse-off products, except oral care products. b) Oral care products. c) Leave-on products. Maximum concentration in ready for use preparation a) 2.5% (acid) b) 1.7% (acid) c) 0.5% (acid)

**Harmonised CLP classification**  
Hazard Class and Category Codes : STOT RE 1 Skin Irrit. 2 Eye Dam. 1 Update : ATP06

**Scientific literature**

- ECHA website - Benzoic acid - Brief Profile - Last updated: 21/12/2021
- SCCNFP/0532/01
- SCCP/0891/05
- SCCNFP/0125/99
- IJT 36(Suppl. 3):5-30, 2017
- IJT 20(suppl 3):23-50, 2001

Full Monography





←

## BENZOIC ACID

CAS: 65-85-0

Cosmetic function  
Fragrance Preservative pH Adjusters

EINECS  
200-618-2

SMILES  
OC(=O)C1=CC=CC=C1

Impurities  
-

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Created  
03/07/2021 00:00

Last modified  
01/01/2022 12:00

Overview
Substance Information
Toxicity
Attached Documentation (1)
Versions (2)

### Physical / chemical properties

MW  
122.12 g/mol

Log  $K_{ow}$  (Octanol-Water)  
1.88

Melting point  
122.4 °C

Boiling point  
172.8 - 249.2 °C @ 79.993 - 1 013.25 hPa

Water solubility  
3.5 g/L @ 25 °C

Other data  
-

### Bioavailability

Summary  
-

Dermal absorption  
50.0%

Oral bioavailability  
100.0%

Inhalatory bioavailability  
100.0%


### Main impurities

Expected impurities

Quantitative impurities

INCI	Estimated impurity (%)






**BENZOIC ACID**  
CAS: 65-85-0

Cosmetic function  
Fragrance Preservative pH Adjusters

EINECS  
200-618-2

SMILES  
OC(=O)C1=CC=CC=C1

Impurities  
-

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Created  
03/07/2021 00:00

Last modified  
01/01/2022 12:00

Overview
Substance Information
Toxicity
Attached Documentation (1)
Versions (2)

### Local toxicity: literature (in vivo/in vitro) - in silico

**Skin irritation**  
SCCP/0891/05: Scarified skin : -7.5 % in ethanol : moderate irritant -15.0 % in ethanol : marked irritant with erosions Normal skin : 30 % in ethanol : lowest irritant concentration Ref. : 16, 17

**Eye irritation**  
SCCP/0891/05: Test was carried out according to OECD guideline 405. Results : mild irritation on rabbit eyes. Ref. : 20, citation in 45 Instillation of 50 mg into the conjunctival sac of 2 rabbits. Results : moderate irritation. Ref. : 21, citation in 45

**Skin sensitization**  
SCCP/0891/05: Mouse Ear Swelling test: 20% benzoic acid in acetone for induction and challenge. No sensitising effects. Ref. : 13 Patch test (48 h/occlusive) according to the ICDRG recommendations: 5 % benzoic acid in petrolatum, 627 patients. 8 patients showed positive reactions (1.3% of the tested). Some reactions may be interpreted as allergic but may have been irritant. Ref. : 14 25 human volunteers were given five 48 h patch tests (during the 10 d period) with 2 % benzoic acid in petrolatum. None gave positive reactions when challenged 10-14 d after the induction phase by a final 48 h closed patch test with 2 % benzoic acid in petrolatum (only abstract available). Ref. : 23, cited in 46 10 persons allergic to benzoyl peroxide were tested by a 48 h patch test with 5 % benzoic acid in a petrolatum. No reactions at 48, 72 and 96 h. Ref. : 24 5203 patients with suspected contact dermatitis were patch tested with benzoic acid (no details were given). 34 patients (0.7 %) showed allergic reactions. Ref. : 25

**Photo-induced toxicity**  
-

**Dermal sensitization**  
-

### Systemic toxicity: literature (in vivo/in vitro) - in silico

**POD**  
ECHA: Reproductive toxicity NOAEL: 175 mg/kg bw/day (subacute, rat, oral)

**Selected POD value**  
175.0

**Repeated toxicity data**  
ECHA:

**Oral**  
NOAEL (rat): 905 - 2 620 mg/kg bw/day  
NOAEL (mouse): 3 571 mg/kg bw/day

**Inhalation**  
NOAEL (rat): 250 mg/m<sup>3</sup> air  
NOAEC (rat): 25 mg/m<sup>3</sup> air

**Dermal**  
NOAEL (rabbit): 2 500 mg/kg bw/day  
SCCP/0891/05  
NOAEL 500 mg/kg bw/d from a 4-generation study (selected by SCF)

**Acute toxicity data**  
ECHA:

Selezionando un ingrediente, si possono visionare tutti i **dettagli scientifici d'interesse**, così da avere uno scenario completo.

Nella tab *toxicity* troverete dati di letteratura (*in vivo/in vitro*) e dati *in silico* sulla tossicità locale, acuta e sistemica.





## Ingredient monography

BENZOIC ACID

**INCI:** BENZOIC ACID

**CAS:** 65-85-0

**EINECS:** 200-618-2

**SMILES:** OC(=O)C1=CC=CC=C1

**Chemical structure:**

**Cosmetic functions:** Fragrance

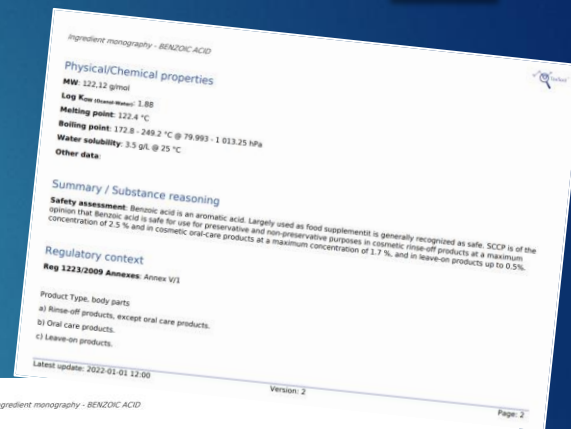
Preservative

pH Adjusters

Latest update: 2022-01-01 12:00

Version: 2

Exported: 2022-07-13 15:53



# ToxTool

The innovative easy-to-use platform for *cosmetics* safety assessment

# ToxTool

Nuove richieste ingredienti

ToxTool®: online toxicological database

The screenshot displays the ToxTool web interface. On the left, the 'Tox DB' search results page shows a search for 'shea butter ethyl esters' and a message: 'Currently, no ingredient with INCI shea butter ethyl esters is present in the ToxTool database. If you believe that the ingredient, in the exact format you entered, is an INCI name that should be included in the ToxTool database, please click on the "Request ingredient" link below. You will be asked for any further information available and the ToxTool team will examine your request. We will keep you posted about your submission.' A 'Request ingredient' link is visible at the bottom of this section.

On the right, the 'My requests' page shows a search for 'shea butter ethyl esters' and a table with one request entry:

INCI	Annotation	Response	State	Created by	Created on ↓
shea butter ethyl esters			Sent	marco.pirozzi	2022-07-13 13:55

The interface also includes a user profile for 'marco.pirozzi' and navigation options for 'Toxicological DB' (3948 items), 'Products' (2 items), and 'My requests' (1 item).

**Un ingrediente cosmetico di vostro interesse non è presente?**

**Nessun problema:** richiedetelo al nostro team tecnico!

Ogni richiesta verrà tracciata con uno stato di lavoro facilmente visionabile sul menù di sinistra. In automatico verrete avvisati quando l'ingrediente verrà caricato sul nostro database.

**Senza costi aggiuntivi.**



**prova**  
Cosmetica Italia Servizi

In progress Finalize

Liquid foundation  
Exposure: dermal

Estimated daily amount applied (g/day)  
3.08

Area for application (cm²)  
565

Retention factor  
1.0

Daily Exposure (g/day)  
3.08

marco.pirozzi

Creation  
Last modified  
marco.pirozzi, 24/06/2022 22:55

Product data | Documentation (0) | Versions (0)

Formula | Tox data | Exp-Dermal | Exp-Oral | Exp-Inhal

INCI	100.0000%	CAS	EINECS	Function	Ingredient reasoning	Possible Impurities	EU Reg 1223/2009 Annexes
AQUA	70.0000 %	7732-18-5	231-791-2	Solvent	Aqua is the most common biological solven...	-	-
HOMOSALATE	20.4500 %	118-56-9	204-260-8	skin conditioning, UV absorber, UV filter	Homosalate caused no signs of sensitizatio...		AnnexVI/3 Maximum con
GLYCERIN	1.9755 %	56-81-5	200-289-5	Denaturant Hair conditioning Humectant O...	Glycerin is a naturally occurring alcohol co...	Diethylene glycol	
ASCORBYL STEARATE	2.6870 %	25395-66-8	246-944-9	Antioxidant	Ascorbyl Stearate is produced by the reacti...	palmitic acid, L-ascorbyl ste...	
ARBUTIN	4.8875 %	497-76-7	207-850-3	antioxidant, bleaching, skin conditioning	Arbutin is a glycoside. The skin irritation stu...		

acorbil stearate 30.45 + Import ingredients from Excel

Downloading your formula

INCI	100.0000% <span>×</span>	POD value (mg/Kg bw/day)	Dermal absorption	External Dermal Exposure (mg/day)	Formula			Tox data			Exp-Dermal	Exp-Oral	Exp-Inhal			
					SED (mg/Kg bw/day)			MoS			Adult (60 Kg)	Baby (1-3 yr, 12 Kg)	Newborn (0-1 yr, 6 Kg)	Adult (60 Kg)	Baby (1-3 yr, 12 Kg)	Newborn (0-1 yr, 6 Kg)
					Adult (60 Kg)	Baby (1-3 yr, 12 Kg)	Newborn (0-1 yr, 6 Kg)	Adult (60 Kg)	Baby (1-3 yr, 12 Kg)	Newborn (0-1 yr, 6 Kg)						
AQUA (WATER)	80.9160 % <span>×</span>		50.0%	1213.740	10.1145	50.5725	101.1450	-	-	-						
CETEARYL ALCOHOL	6.3500 % <span>×</span>	750.0	1.0%	95.250	0.0159	0.0794	0.1588	47244.0945	9448.8189	4724.4094						
CAPRYLIC/CAPRIC TRIGLYCERIDE	3.0000 % <span>×</span>	5000.0	50.0%	45.000	0.3750	1.8750	3.7500	13333.3333	2666.6667	1333.3333						
ORYZA SATIVA (RICE) BRAN OIL	2.8000 % <span>×</span>		50.0%	42.000	0.3500	1.7500	3.5000	-	-	-						
GLYCERYL STEARATE	2.3500 % <span>×</span>	1000.0	40.0%	35.250	0.2350	1.1750	2.3500	4255.3191	851.0638	425.5319						
STEARIC ACID	1.3000 % <span>×</span>	1000.0	50.0%	19.500	0.1625	0.8125	1.6250	6153.8462	1230.7692	615.3846						
PHENOXYETHANOL	0.9000 % <span>×</span>	357.0	100.0%	13.500	0.2250	1.1250	2.2500	1586.6667	317.3333	158.6667						
SODIUM LAUROYL GLUTAMATE	0.7500 % <span>×</span>	1200.0	50.0%	11.250	0.0938	0.4688	0.9375	12800.0000	2560.0000	1280.0000						
PARFUM (FRAGRANCE)	0.4416 % <span>×</span>		50.0%	6.624	0.0552	0.2760	0.5520	-	-	-						
XANTHAN GUM	0.4000 % <span>×</span>	250.0	10.0%	6.000	0.0100	0.0500	0.1000	25000.0000	5000.0000	2500.0000						



## Exportable Reports

Exposure and risk characterisation

Hazard identification

Raw data

Ingredients monography (summary)

Download all documents

### Exposure and risk characterisation Target population adult (60 Kg)

INCI	%	External Dermal Exposure (mg/day)	POD value (mg/kg bw/d)	SED derma 1 (mg/ Kg bw/d)	MoS dermal	SED oral (mg/ Kg bw/d)	MoS oral	SED inhalatio n (mg/ Kg bw/d)	MoS inhalatio n	Regulatory status	Substance Reasoning
AQUA (WATER)	80.916	1213.739		10.114	0.0000	20.229	0.0000	0.0000	NaN	There is no harmonised classification.	Aqua (Water) is the most common biological solvent found in all living organisms. Widely used for all cosmetic uses, it can be considered safe when used as cosmetic ingredient. Cetearyl Alcohol is a

### Hazard identification CETEARYL ALCOHOL

Ingredient data  
INCI: CETEARYL ALCOHOL  
CAS: 67762-27-0 / 8005-44-5  
EINECS: 267-008-6 / -  
Impurities: PAHs

### Local toxicity

Skin irritation	Eye Irritation	Skin sensitization	Photo-Induced toxicity
Additionally, the classification provided by companies to ECHA in CLP notifications identifies that this substance causes skin irritation.	Additionally, the classification provided by companies to ECHA in CLP notifications identifies that this substance causes serious eye irritation.	No evidence of sensitization was produced.	

### Systemic toxicity

Repeated Dose Toxicity Data	Acute Toxicity Data	Toxicity to Reproduction Data	Genetic Toxicity / Carcinogenicity Data	Endocrine activity	Organospecific Toxicity	TTC
<p>Repeated dose toxicity</p> <p>Oral route - systemic effects:</p> <p>No adverse effect observed NOAEL 750 mg/kg bw/day (subchronic, rat)</p> <p>Oral route - systemic effects:</p> <p>No adverse effect observed NOAEL 1 000 mg/kg bw/day (subacute, rat)</p>	<p>Acute toxicity Oral route:</p> <p>No adverse effect observed NOAEL 1 000 mg/kg bw (subchronic, rat)</p> <p>Acute toxicity Inhalation route:</p> <p>No adverse effect observed NOAEL 1 000 mg/m<sup>3</sup> (subacute, rat)</p>	<p>Effect on fertility Oral route:</p> <p>No adverse effect observed NOAEL 1 000 mg/kg bw (chronic, rat)</p> <p>Effect on reproduction Dermal route:</p> <p>No adverse effect observed NOAEL 45.55 mg/kg bw/day (chronic, rat)</p> <p>Inhalation route:</p>	<p>Genotoxicity - in vitro</p> <p>No adverse effect observed (negative)</p> <p>Genotoxicity - in vivo</p> <p>No adverse effect observed (negative)</p> <p>Carcinogenicity</p> <p>Oral route:</p> <p>No adverse effect observed NOAEL 931.06 mg/kg bw/day (chronic, rat)</p>			<p>Classification according Cramer class Low (Class 1) TTC according Cramer Classification: 0.03 mg/kg bw/day</p>

- Ingredients monography
  - Exposure and risk characterisation
  - Hazard identification
  - Raw data
- 005\_CAPRYLIC-CAPRIC TRIGLYCERIDE
  - 006\_ORYZA SATIVA (RICE) BRAN OIL
  - 007\_GLYCERYL STEARATE
  - 008\_GLYCERYL STEARATE
  - 009\_STEARIC ACID
  - 010\_STEARIC ACID
  - 011\_PHENOXYETHANOL
  - 012\_SODIUM LAUROYL GLUTAMATE
  - 013\_PARFUM (FRAGRANCE)
  - 014\_XANTHAN GUM
  - 015\_DCOIPHERYL ACETATE
  - 016\_COCOS NUCIFERA (COCONUT) OIL

inci	elieca	function_description	safety_assessment	scientific_literature
BENZYL ALCOHOL	202.485-3	Purifying Preservative/Solvent Viscosity Controlling	<p>preservative (p to 70) or can be a volatile component of fragrances and essential oils. It is listed in Annex 1B of the 12th amendment commonly known as allergens.</p> <p>CFR Expert panel concluded that Benzyl Alcohol is safe when used as cosmetic ingredient up to 10% in general and up to 10% in hair dress.</p> <p>When used as a fragrance component it can be considered safe when in compliance with IFRA standards.</p>	<p>09020022</p> <p>J. Am. Assoc. of Food and Chemical Toxicology 14 (1918) 15-24</p> <p>UT 20 (sept 1922-30, 2008)</p> <p>UT 30 (sept 1930-30, 2007)</p> <p>SCCNF(94)5401</p> <p>SCCNF(94)5401 - Opinion concerning Essential Oils</p> <p>SCCNF(94)5701 - Opinion concerning Fragrance Allergens</p>
CITRIC ACID	206.084-1	Buffing/Chelating Masking	<p>Organic Acid largely used in food (not E230).</p> <p>The CIR Expert Panel concluded that citric acids are safe when used as cosmetic ingredients at concentrations up to 10%.</p> <p>According to the SCCS Opinion on citric acid and other citrate, 10 October 2010 the low availability of the ingredients in the cosmetics formulations may be found in cosmetics as well as in non-cosmetic products such as household cleaners and detergents. It was reported to be a fragrance ingredient used in many fragrance mixtures. It had been reported to cause severe rash and dermatitis. Acute oral toxicity The LD50 values in female and male rats/Ratfish were determined to be 3840 mg/kg bw and 4070 mg/kg bw respectively. Skin irritation: Under the conditions of the in vivo study,</p>	<p>ECHA Website - Citric Acid Ester Phthalate - Last updated: 04/04/2012</p> <p>SCCS (Scientific Steering Committee) Citric Acid for High Production Volume Chemicals (2004) (02) - UT 30 (sept 2003-04, 2004)</p> <p>SCCS (Scientific Committee on Consumer Safety), Opinion on citric acid and other citrate, 10 October 2010</p> <p>SCCS (9/19) Final version of October 2010: Scientific Committee on Consumer Safety (SCCS) OPINION ON PHENOXYETHANOL</p> <p>J. Am. Coll. Toxicol. Vol. 2 (1993) pp 255-60</p> <p>* ANEM report on phenoxyethanol - UT 30 (sept 1922-30, 2008)</p> <p>* ECHA Website - 2-phenoxyethanol - Last updated: 17/02/2012</p>
PHENOXYETHANOL	204.583-3	Preservative		

Tutta la documentazione viene esportata istantaneamente, così da poterla allegare facilmente alla propria documentazione informativa sul prodotto e consultarla nel dettaglio in caso d'interesse.

**Esposizione, caratterizzazione del rischio, identificazione dei pericoli, monografie di tutti gli ingredienti e tutti i dati puntuali in formato excel dell'intera formula.**



# ToxTool

The innovative easy-to-use platform for *cosmetics* safety assessment

# ToxTool

Protection

ToxTool®: online toxicological database





## Exposure and risk characterisation

### Cosmetica Italia Servizi

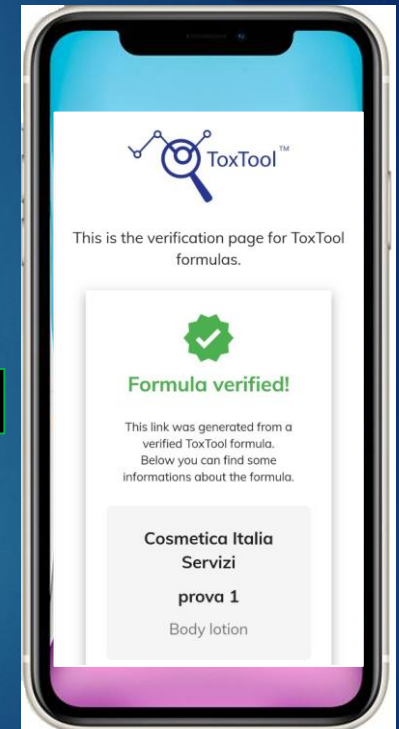
#### prova 1


Version 1  
2022-07-13 16:52

<b>Product type:</b> Body lotion	<b>Dermal exposure:</b> applicable
<b>Daily amount applied <math>q_x</math> (g/d):</b> 1.5	<b>Oral exposure:</b> unlikely
<b>Retention factor:</b> 1.0	<b>Inhalation exposure:</b> unlikely




QR Security code





This is the verification page for ToxTool formulas.

  
**Formula verified!**

This link was generated from a verified ToxTool formula.  
Below you can find some informations about the formula.

**Cosmetica Italia Servizi**  
**prova 1**  
Body lotion




toxtool.eu






# Are you Ready?

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