

Product Number **D004**
Revision Number **RN4.0**

Revision Date 2 December 2021

1. Product and Company Identification

Product Name	1,3-Dimethyl-4,5-diphenyl-2-[(2-oxopropyl)thio]imidazolium trifluorosulfonic acid salt L-683.685		
CAS-No.	No data available		
EC-No.	No data available		
REACH No.	The substance does not require registration according to Regulation (EC) No 1907/2006 [REACH].		
Identified Uses	Inhibitor for transglutaminase. This material is intended for research purposes only.		
Uses Advised Against	This product is not intended for food, drug, household, agricultural or cosmetic use. Its use must be supervised by a technically qualified individual experienced in handling potentially hazardous chemicals.		
Manufacturer/Supplier	Zedira GmbH Rösslerstr. 83 64293 Darmstadt Germany	Tel. +49 6151 66628-0 Fax. +49 6151 66628-19	
Emergency Call	+49 6131 19240 (Poison Control Center Mainz)		

2. Hazards Identification

2.1 Classification of the substance or mixture

Not a hazardous substance or mixture according to Regulation (EC) No. 1272/2008.

2.2 Label elements

Not a hazardous substance or mixture according to Regulation (EC) No. 1272/2008.

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

3. Composition / Information on Components

IUPAC	1,3-Dimethyl-2-(2-oxopropylthio)-4,5-diphenyl-1H-imidazol-3-ium trifluoromethanesulfonate
Molecular Formula	C ₂₁ H ₂₁ F ₃ N ₂ O ₄ S ₂ (free cation: C ₂₀ H ₂₁ N ₂ OS ⁺)
Molecular Weight	486.53 (free cation: 337.46)

4. First Aid Measures

Skin Contact: If skin contact occurs, wash off immediately with plenty of water for at least 15 minutes.
If skin irritation persists, call a physician.

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Eye Contact: After eye contact, rinse immediately with plenty of water (also under the eyelids) for at least 15 minutes, get medical attention.

Inhalation: If inhaled, move individual to fresh air and seek medical advice.

Ingestion: If swallowed, wash mouth with water and seek medical advice.

Avoid prolonged or repeated exposure. Use personal protective equipment as required.

5. Fire Fighting Measures

Use carbon dioxide extinguisher, dry chemical powder, or appropriate foam extinguisher.

6. Accidental Release Measures

Use appropriate personal protective equipment and methods to clean up spilled substances promptly. Absorb spill onto an appropriate material. Collect and dispose of all waste in accordance with applicable laws.

Avoid dust formation. Avoid breathing vapors, mist, or gas. Ensure adequate ventilation. Remove all sources of ignition.

Avoid release into the environment.

7. Handling and Storage

Store at -20°C, desiccate. Shipping is possible at ambient temperature.

Avoid contact with eyes, skin, or on clothing. Wear personal protective equipment/face protection. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces, and sources of ignition. Provide appropriate exhaust ventilation at places where dust, aerosols or vapors are formed. Reduce the release of the substance or mixture to the environment, avoid spills, keep away from drains.

Handle in accordance with appropriate industrial hygiene and safety practice. Keep away from food. Do not eat, drink, or smoke in work areas. Wash hands after use and remove contaminated clothing and protective equipment before entering eating areas.

8. Exposure Controls and Personal Protection

Wear appropriate gloves, protective clothing and eyewear and follow safe laboratory practices.

This product does not contain any hazardous materials with occupational exposure limits established by the region-specific regulatory bodies.

Use under a chemical fume hood, if appropriate. Ensure that eyewash stations and safety showers are close to the workstation location. Use explosion-proof electrical/ventilating/lighting/equipment.

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN 166.

Wear appropriate protective gloves and clothing to prevent skin exposure.

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Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Handle in accordance with good industrial hygiene and safety practice.

9. Physical and Chemical Properties

Appearance	Off white solid
Odor	Odourless
Melting point/freezing point	No data available
Boiling point	No data available
Flammability	No data available
Lower/upper explosion limit	No data available
Flashpoint	No data available
Auto-ignition temperature	No data available
Decomposition temperature	No data available
pH	No data available
Kinematic viscosity	No data available
Solubility	400 µM in 2% (v/v) DMSO / aqueous buffers
Partition coefficient	No data available
Vapour pressure	No data available
Density	No data available
Specific Gravity	No data available
Relative vapour density	No data available
Particle characteristics	No data available

10. Stability and Reactivity

Conditions to be Avoided: Avoid direct sunlight, moisture, conditions that might generate heat and dispersion.

Substances to be Avoided: No studies have been conducted. Avoid contact with strong oxidizing or reducing agents.

11. Toxicological Information

Acute toxicity	No data available
Skin corrosion/irritation	No data available
Eye damage/irritation	No data available
Respiratory or skin sensitization	No data available
Germ cell mutagenicity	No data available
Carcinogenicity	IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible, or confirmed human carcinogen by IARC.
Reproductive toxicity	No data available
Aspiration hazard	No data available
Specific target organ toxicity	
- single exposure	No data available
- repeated exposure	No data available
RTECS Number	No data available

12. Ecological Information

No information is available about the potential of this material to produce adverse environmental effects such as ecotoxicity, persistence and degradability, bioaccumulation, mobility (soil) or other adverse effects.

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Results of PBT and vPvB assessment: No data available.

13. Disposal Considerations

The generation of waste should be avoided or minimized wherever possible. Disposal of this product, solutions and any by-products should always comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Dispose of surplus and nonrecyclable products via a licensed waste disposal contractor. Waste should not be disposed of untreated to the sewer unless fully compliant with the requirements of all authorities with jurisdiction.

14. Transport Information

Land transport (ADR/RID)	Not regulated
Inland waterway transport (ADN)	Not regulated
Sea transport (IMDG)	Not regulated
Air transport (ICAO-TI / IATA-DGR)	Not regulated
Environmental hazards	No hazards identified
Special precautions for user	No special precautions required
Proper Shipping Name	Non-dangerous goods
Maritime transport in bulk according to IMO instruments:	Not applicable, packaged goods

15. Regulations

This material safety data sheet (MSDS) complies with the requirements of Regulation (EC) No. 1907/2006 including amendment (EU) 2020/878.

Toxic Substances Control Act (TSCA): This substance is not subject to TSCA requirements.

Chemical safety assessment: For this product, a chemical safety assessment was not carried out.

16. Other Information

The above information is correct to the best of our knowledge. Users should make independent decisions regarding completeness of the information based on all sources available. Zedira GmbH shall not be held liable for any damage resulting from handling or contact with the above product.