MATERIAL SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Date of issue: 02/05/2013 Version 1.0

SECTION 1. Identification

Product identifier

Product number	811731
Product name	Crown ether/Dibenzo-18-crown-6 for synthesis

Relevant identified uses of the substance or mixture and uses advised against

Identified uses	Chemical for synthesis

Details of the supplier of the safety data sheet

Company	EMD Millipore Corporation | 290 Concord Road, Billerica, MA 01821, United States of America | SDS Phone Support: +1-978-715-1335 | General Inquiries: +1-978-715-4321 | Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5) e-mail: mm_sds@merckgroup.com
Emergency telephone	800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. Hazards identification

GHS-Labeling

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

OSHA Hazards

While this material is not considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200), this MSDS contains valuable information critical to the safe handling and proper use of the product. This MSDS should be retained and available for employees and other users of this product.

Other hazards

None known.

The following percentage of the mixture consists of ingredient(s) with unknown acute toxicity: 100 %

SECTION 3. Composition/information on ingredients

Formula	$C_{20}H_{24}O_6$ (Hill)
CAS-No.	14187-32-7
Molar mass	360.41 g/mol

Remarks	No hazardous ingredients according to the OSHA Hazard Communication Standard 29 CFR 1910.1200.

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air.

Skin contact

After skin contact: wash off with plenty of water. Remove contaminated clothing.

Eye contact

After eye contact: rinse out with plenty of water with the eyelid held wide open. Call in ophthalmologist if necessary.

Ingestion

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

irritant effects, Convulsions

Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media

Water, Carbon dioxide (CO2), Foam, Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Special hazards arising from the substance or mixture

Combustible material, Development of hazardous combustion gases or vapors possible in the event of fire.

Advice for firefighters

Special protective equipment for fire-fighters

In the event of fire, wear self-contained breathing apparatus.

Further information

Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid generation of dusts; do not inhale dusts. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

Environmental precautions
Do not empty into drains.

Methods and materials for containment and cleaning up
Cover drains. Collect, bind, and pump off spills.
Observe possible material restrictions (see sections 7 and 10).
Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7. Handling and storage

Precautions for safe handling
Observe label precautions.

Conditions for safe storage, including any incompatibilities
Tightly closed. Dry.

Store at +15°C to +25°C (+59°F to +77°F).

SECTION 8. Exposure controls/personal protection

Exposure limit(s)
Contains no substances with occupational exposure limit values.

Engineering measures
Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

Individual protection measures
Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures
Change contaminated clothing. Wash hands after working with substance.

Eye/face protection
Safety glasses

Hand protection
Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Respiratory protection
required when dusts are generated.
Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

SECTION 9. Physical and chemical properties

Physical state	powder, finecrystalline
Color	beige

Odor	No strong odor known.
Odor Threshold	No information available.
pH	No information available.
Melting point	158 - 161 °C
Boiling point/boiling range	716 - 723 °F (380 - 384 °C) at 680 hPa
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapor pressure	No information available.
Relative vapor density	No information available.
Relative density	No information available.
Water solubility	0.007 g/l at 77 °F (25 °C)
Partition coefficient: n-octanol/water	log Pow: 2.2 (experimental) (Lit.) Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	No information available.

SECTION 10. Stability and reactivity

Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

Chemical stability
The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions
Violent reactions possible with:

Strong oxidizing agents, Strong acids

Conditions to avoid
Strong heating.

Incompatible materials
no information available

Hazardous decomposition products
no information available

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure
Eye contact, Skin contact, Ingestion

Acute oral toxicity
LD50 rat: 2,600 mg/kg (RTECS)
Symptoms: Convulsions

Eye irritation
rabbit
slight irritation (RTECS)

Specific target organ systemic toxicity - single exposure
The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ systemic toxicity - repeated exposure
The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard
Regarding the available data the classification criteria are not fulfilled.

Carcinogenicity

IARC	No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
OSHA	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
NTP	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
ACGIH	No ingredient of this product present at levels greater than or

equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

Further information

Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.
Further data:
Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

No information available.

Persistence and degradability

No information available.

Bioaccumulative potential

Partition coefficient: n-octanol/water
log Pow: 2.2
(experimental)
(Lit.)

Bioaccumulation is not expected (log Pow <1).

Mobility in soil

No information available.

Other adverse effects

Additional ecological information
We have no quantitative data concerning the ecological effects of this product.
Further information on ecology
Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

SECTION 14. Transport information

Land transport (DOT)

Not classified as dangerous in the meaning of transport regulations.

Air transport (IATA)

Not classified as dangerous in the meaning of transport regulations.

Sea transport (IMDG)

Not classified as dangerous in the meaning of transport regulations.

SECTION 15. Regulatory information

United States of America

OSHA Hazards

No OSHA Hazards

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

SARA 311/312 Hazards

No SARA Hazards

SARA 313

SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 302

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

Massachusetts Right To Know

Remarks

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know

Ingredients

dibenzo[a,j]-1,4,7,10,13,16-hexaoxacyclooctadeca-2,11-diene

New Jersey Right To Know

Ingredients

dibenzo[a,j]-1,4,7,10,13,16-hexaoxacyclooctadeca-2,11-diene

Notification status

TSCA:	On TSCA Inventory
DSL:	This product contains one or several components listed in the Canadian NDSL. *Ingredients* dibenzo[a,j]-1,4,7,10,13,16-hexaoxacyclooctadeca-2,11-diene

SECTION 16. Other information

Training advice

Provide adequate information, instruction and training for operators.

Key or legend to abbreviations and acronyms used in the safety data sheet
Used abbreviations and acronyms can be looked up at www.wikipedia.org.

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The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.
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