

## SAFETY DATA SHEET

Version 6.9  
Revision Date 09/07/2024  
Print Date 09/08/2024**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**Product name : 2-Benzyl-2-(dimethylamino)-4'-  
morpholinobutyrophenoneProduct Number : 405647  
Brand : Aldrich  
Index-No. : 606-047-00-9  
CAS-No. : 119313-12-1**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&amp;D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&amp;D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

**1.3 Details of the supplier of the safety data sheet**Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATESTelephone : +1 314 771-5765  
Fax : +1 800 325-5052**1.4 Emergency telephone**Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**Reproductive toxicity (Category 1B), H360  
Short-term (acute) aquatic hazard (Category 1), H400

Aldrich - 405647

Page 1 of 11

Long-term (chronic) aquatic hazard (Category 1), H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H360

May damage fertility or the unborn child.

H410

Very toxic to aquatic life with long lasting effects.

Precautionary Statements

P201

Obtain special instructions before use.

P202

Do not handle until all safety precautions have been read and understood.

P273

Avoid release to the environment.

P280

Wear protective gloves/ protective clothing/ eye protection/ face protection.

P308 + P313

IF exposed or concerned: Get medical advice/ attention.

P391

Collect spillage.

P405

Store locked up.

P501

Dispose of contents/ container to an approved waste disposal plant.

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

Formula :  $C_{23}H_{30}N_2O_2$   
Molecular weight : 366.50 g/mol  
CAS-No. : 119313-12-1  
EC-No. : 404-360-3  
Index-No. : 606-047-00-9

Component	Classification	Concentration
<b>2-benzyl-2-dimethylamino-4-morpholinobutyrophenone</b>		
	Repr. 1B; Aquatic Acute 1; Aquatic Chronic 1; H360, H400, H410 M-Factor - Aquatic Acute: 10 M-Factor - Aquatic Chronic: 10	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

---

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Call in physician.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

#### If swallowed

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

### 4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

### 4.3 Indication of any immediate medical attention and special treatment needed

No data available

---

## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

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

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

### 5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

### 5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

---

## **SECTION 6: Accidental release measures**

### **6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

### **6.2 Environmental precautions**

Do not let product enter drains.

### **6.3 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 carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

### **6.4 Reference to other sections**

For disposal see section 13.

---

## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

#### **Advice on safe handling**

Work under hood. Do not inhale substance/mixture.

#### **Hygiene measures**

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

### **7.2 Conditions for safe storage, including any incompatibilities**

#### **Storage conditions**

Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

#### **Storage class**

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

### **7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

---

## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Ingredients with workplace control parameters**

Contains no substances with occupational exposure limit values.

## 8.2 Exposure controls

### Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

### Personal protective equipment

#### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

#### Skin protection

Handle with impervious gloves.

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

#### Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested:KCL 741 Dermatril® L

#### Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested:KCL 741 Dermatril® L

#### Body Protection

protective clothing

#### Respiratory protection

Recommended Filter type: Filter type P3

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.  
required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

#### Control of environmental exposure

Do not let product enter drains.

---

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- a) Appearance                      Form: powder

b) Odor	odorless
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/ range: 116 - 119 °C (241 - 246 °F) - lit.
f) Initial boiling point and boiling range	No data available
g) Flash point	113 °C (235 °F)
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	1.21 g/cm <sup>3</sup> at 20 °C (68 °F)
Relative density	No data available
n) Water solubility	0.0059 g/l at 20 °C (68 °F) at 6.75 hPa
o) Partition coefficient: n-octanol/water	log Pow: 2.91 at 25 °C (77 °F) - Bioaccumulation is not expected.
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

## 9.2 Other safety information

Surface tension 59.1 mN/m at 20 °C (68 °F)

---

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

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.

## 10.2 Chemical stability

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

## 10.3 Possibility of hazardous reactions

No data available

## 10.4 Conditions to avoid

Strong heating.

## 10.5 Incompatible materials

Strong oxidizing agents, Strong acids

## 10.6 Hazardous decomposition products

In the event of fire: see section 5

---

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - male and female - > 5,000 mg/kg

(OECD Test Guideline 401)

Inhalation: No data available

LD50 Dermal - Rat - male and female - > 2,000 mg/kg

(OECD Test Guideline 402)

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

(OECD Test Guideline 404)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

#### Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

#### Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Aldrich - 405647

Page 7 of 11

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

### **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.

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.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

### **Reproductive toxicity**

May damage the unborn child.

### **Specific target organ toxicity - single exposure**

No data available

### **Specific target organ toxicity - repeated exposure**

No data available

### **Aspiration hazard**

No data available

## **11.2 Additional Information**

RTECS: EL7755000

Anorexia., Liver injury may occur., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Anorexia., Liver injury may occur., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

---

## **SECTION 12: Ecological information**

### **12.1 Toxicity**

Toxicity to fish	semi-static test LC50 - Danio rerio (zebra fish) - > 0.142 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	semi-static test NOEC - Daphnia magna (Water flea) - 0.21 mg/l - 21 h
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata - > 2 mg/l - 72 h (OECD Test Guideline 201) static test NOEC - Pseudokirchneriella subcapitata - 0.5 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test - activated sludge - > 100 mg/l - 0.5 h (OECD Test Guideline 209)

### **12.2 Persistence and degradability**

Biodegradability aerobic - Exposure time 28 d  
Result: 3 % - Not readily biodegradable.

Aldrich - 405647

Page 8 of 11



**12.3 Bioaccumulative potential**

No data available

**12.4 Mobility in soil**

No data available

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

**12.6 Endocrine disrupting properties**

No data available

**12.7 Other adverse effects**

No data available

---

**SECTION 13: Disposal considerations**

**13.1 Waste treatment methods**

**Product**

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

---

**SECTION 14: Transport information**

**DOT (US)**

Not dangerous goods

**IMDG**

UN number: 3077 Class: 9 Packing group: III EMS-No: F-A, S-F  
Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (2-benzyl-2-dimethylamino-4-morpholinobutyrophenone)  
Marine pollutant : yes  
Marine pollutant : no

**IATA**

UN number: 3077 Class: 9 Packing group: III  
Proper shipping name: Environmentally hazardous substance, solid, n.o.s. (2-benzyl-2-dimethylamino-4-morpholinobutyrophenone)

**Further information**

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids. Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

---

## SECTION 15: Regulatory information

### **CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

### **SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

### **SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : No SARA Hazards

**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.

## **US State Regulations**

### **Massachusetts Right To Know**

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

### **Maine Chemicals of High Concern**

Product does not contain any listed chemicals

### **Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

### **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

### **The ingredients of this product are reported in the following inventories:**

**TSCA** : All substances listed as active on the TSCA inventory

### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

---

## SECTION 16: Other information

### **Further information**

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact

with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

Version: 6.9

Revision Date: 09/07/2024

Print Date: 09/08/2024