

## Chemical Safety Data Sheet MSDS / SDS

**BAY 11-7085**Revision Date:2023-12-07 Revision Number:1

---

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : BAY 11-7085  
CBnumber : CB0675833  
CAS : 196309-76-9  
Synonyms : BAY 11-7085,(2E)-3-[[4-(1,1-DIMETHYLETHYL)PHENYL]SULFONYL]-2-PROPENITRILE

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 400-158-6606

---

**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)

**Precautionary statements**

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.  
Continuerinsing.  
P405 Store locked up.

**Hazard statements**

H302 Harmful if swallowed  
H315 Causes skin irritation  
H319 Causes serious eye irritation  
H335 May cause respiratory irritation

---

**SECTION 3: Composition/information on ingredients**

## Substance

Product name	: BAY 11-7085
Synonyms	: BAY 11-7085,(2E)-3-[[4-(1,1-DIMETHYLETHYL)PHENYL]SULFONYL]-2-PROPENITRILE
CAS	: 196309-76-9
MF	: C13H15NO2S
MW	: 249.33

---

## SECTION 4: First aid measures

### Description of first aid measures

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration.

#### In case of skin contact

Wash off with soap and plenty of water.

#### In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water.

### 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

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

No data available

---

## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

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

Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), Sulphur oxides

#### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### Further information

No data available

### NFPA 704





■ HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

■ FIRE 0 Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand. Materials that will not burn in air when exposed to a temperature of 820 °C (1,500 °F) for a period of 5 minutes.(e.g. Carbon tetrachloride)

■ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium,[N2](#))

□ SPEC.  
HAZ.

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing vapours, mist or gas. For personal protection see section 8.

### Environmental precautions

Do not let product enter drains.

### Methods and materials for containment and cleaning up

Sweep up and shovel. Keep in suitable, closed containers for disposal.

### Reference to other sections

For disposal see section 13.

## SECTION 7: Handling and storage

### Precautions for safe handling

Provide appropriate exhaust ventilation at places where dust is formed.Normal measures for preventive fire protection.

For precautions see section 2.2.

### Conditions for safe storage, including any incompatibilities

Store in cool place. Keep container tightly closed in a dry and well-ventilated place.

### 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

### control parameter

#### Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

### Exposure controls

#### Appropriate engineering controls

General industrial hygiene practice.

#### 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).

##### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

##### Body Protection

Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

##### Control of environmental exposure

Do not let product enter drains.

---

## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	solid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 80 - 82 °C
Initial boiling point and boiling range	No data available
Flash point	200°C
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available

---

Vapour pressure	No data available
Vapour density	No data available
Relative density	No data available
Water solubility	insoluble
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

---

### **Other safety information**

No data available

---

## SECTION 10: Stability and reactivity

### **Reactivity**

No data available

### **Chemical stability**

Stable under recommended storage conditions.

### **Possibility of hazardous reactions**

No data available

### **Conditions to avoid**

No data available

### **Incompatible materials**

Strong acids, Strong bases

### **Hazardous decomposition products**

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), Sulphur oxides

Other decomposition products - No data available In the event of fire: see section 5

---

## SECTION 11: Toxicological information

### **Information on toxicological effects**

#### **Acute toxicity**

No data available

#### **Skin corrosion/irritation**

No data available

**Serious eye damage/eye irritation**

No data available

**Respiratory or skin sensitisation**

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

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

---

## SECTION 12: Ecological information

**Toxicity**

No data available

**Persistence and degradability**

No data available

**Bioaccumulative potential**

No data available

**Mobility in soil**

No data available

**Results of PBT and vPvB assessment**

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

**Other adverse effects**

No data available

---

## SECTION 13: Disposal considerations

## Waste treatment methods

### Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

### Contaminated packaging

Dispose of as unused product.

---

## SECTION 14: Transport information

### SECTION 14: Transport information

UN number

ADR/RID:IMDG:IATA:ADR/RID:IMDG:IATA:

UN number

ADR/RID:IMDG:IATA:ADR/RID:IMDG:IATA:

IATA:

UN number

ADR/RID:IMDG:IATA:ADR/RID:IMDG:IATA:

UN number

ADR/RID:IMDG:IATA:ADR/RID:IMDG:IATA:

IATA:

### UN number

ADR/RID: 3077 IMDG: 3077 IATA: 3077

ADR/RID: 3271 IMDG: 3271 IATA: 3271

ADR/RID: 2397 IMDG: 2397 IATA: 2397

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: - IMDG: - IATA: -

ADR/RID: 3272 IMDG: 3272 IATA: 3272

ADR/RID: 1665 IMDG: 1665 IATA: 1665

ADR/RID: - IMDG: - IATA: -

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

ADR/RID: - IMDG: - IATA: -

ADR/RID: - IMDG: - IATA: -

### Packaging group

ADR/RID: - IMDG: - IATA: -

ADR/RID: - IMDG: - IATA: -

ADR/RID: III IMDG: III IATA: III

ADR/RID: - IMDG: - IATA: -

ADR/RID: NITROXYLENES, LIQUID IMDG: NITROXYLENES, LIQUID IATA: Nitroxylenes, liquid

ADR/RID: ESTERS, N.O.S. (Ethyl 3-furoate) IMDG: ESTERS, N.O.S. (Ethyl 3-furoate) IATA: Esters, n.o.s. (Ethyl 3-furoate)

ADR/RID: - IMDG: - IATA: -

ADR/RID: III IMDG: III IATA: III

ADR/RID: 3-METHYLBUTAN-2-ONE IMDG: 3-METHYLBUTAN-2-ONE IATA: 3-Methylbutan-2-one

ADR/RID: ETHERS, N.O.S. (2,3-Epoxypropyl isopropyl ether) IMDG: ETHERS, N.O.S. (2,3-Epoxypropyl isopropyl ether) IATA: Ethers, n.o.s. (2,3-Epoxypropyl isopropyl ether)

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (2,7- Bis(bromomethyl)naphthalene) IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (2,7- IATA: Environmentally hazardous substance, solid, n.o.s. Bis(bromomethyl)naphthalene)

### Transport hazard class(es)

(2,7- ADR/RID: 9 IMDG: 9 IATA: 9

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: yes IMDG Marine pollutant: yes IATA: no

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: no IMDG Marine pollutant: no IATA: no

### Special precautions for user

No data available

No data available

No data available

No data available

No data available

ADR/RID: II IMDG: II IATA: II

ADR/RID: III IMDG: III IATA: III

No data available

No data available

ADR/RID: II IMDG: II IATA: II

ADR/RID: III IMDG: III IATA: III

ADR/RID: III IMDG: III IATA: III

### Environmental hazards

ADR/RID: yes IMDG Marine pollutant: yes IATA: yes Bis(bromomethyl)naphthalene) Special precautions for user 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

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: yes IMDG Marine pollutant: yes IATA: no

### Special precautions for user

No data available



No data available

No data available

No data available

---

## SECTION 15: Regulatory information

### Safety, health and environmental regulations/legislation specific for the substance or mixture

#### Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

#### Measures for Environmental Management of New Chemical Substances

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: <https://www.mee.gov.cn/>

EC Inventory:Not Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: <https://echa.europa.eu/>

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: <https://www.epa.govt.nz/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: <https://www.epa.gov/>

Vietnam National Chemical Inventory:Not Listed. website: <https://chemicaldata.gov.vn/>

---

## SECTION 16: Other information

### Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

### References

**[1]** CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

**[2]** ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

**[3]** ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

**[4]** eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)

**[5]** ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

**[6]** Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

**Disclaimer:**

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.