

## SAFETY DATA SHEET

Version 3.6  
Revision Date 09/29/2017  
Print Date 11/10/2018

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**1. PRODUCT AND COMPANY IDENTIFICATION****1.1 Product identifiers**

Product name : XCT790

Product Number : X4753

Brand : Sigma

CAS-No. : 725247-18-7

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

Identified uses : Laboratory chemicals, Synthesis of substances

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

**1.4 Emergency telephone number**

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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**2. HAZARDS IDENTIFICATION****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Chronic aquatic toxicity (Category 4), H413

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

**2.2 GHS Label elements, including precautionary statements**

Pictogram none

Signal word none

Hazard statement(s)

H413 May cause long lasting harmful effects to aquatic life.

Precautionary statement(s)

P273 Avoid release to the environment.

P501 Dispose of contents/ container to an approved waste disposal plant.

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

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**3. COMPOSITION/INFORMATION ON INGREDIENTS****3.1 Substances**

Synonyms : 3-[4-(2,4-Bis-trifluoromethylbenzyloxy)-3-methoxyphenyl]-2-cyano-N-(5-trifluoromethyl-1,3,4-thiadiazol-2-yl)acrylamide

Formula : C<sub>23</sub>H<sub>13</sub>F<sub>9</sub>N<sub>4</sub>O<sub>3</sub>S

Molecular weight : 596.42 g/mol

CAS-No. : 725247-18-7

No components need to be disclosed according to the applicable regulations.  
For the full text of the H-Statements mentioned in this Section, see Section 16.

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#### 4. FIRST AID MEASURES

##### 4.1 Description of first aid measures

###### **General advice**

Consult a physician. Show this safety data sheet to the doctor in attendance.

###### **If inhaled**

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

###### **In case of skin contact**

Wash off with soap and plenty of water. Consult a physician.

###### **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. 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

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#### 5. FIREFIGHTING MEASURES

##### 5.1 Extinguishing media

###### **Suitable extinguishing media**

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

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

No data available

##### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

##### 5.4 Further information

No data available

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#### 6. ACCIDENTAL RELEASE MEASURES

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

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

##### 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

##### 6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

##### 6.4 Reference to other sections

For disposal see section 13.

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#### 7. HANDLING AND STORAGE

##### 7.1 Precautions for safe handling

Provide appropriate exhaust ventilation at places where dust is formed.

For precautions see section 2.2.

## 7.2 Conditions for safe storage, including any incompatibilities

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

Recommended storage temperature 2 - 8 °C

## 7.3 Specific end use(s)

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

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### 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.

##### 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

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |                                            |                   |
|--------------------------------------------|-------------------|
| a) Appearance                              | Form: solid       |
| b) Odour                                   | No data available |
| c) Odour Threshold                         | No data available |
| d) pH                                      | No data available |
| e) Melting point/freezing point            | No data available |
| f) Initial boiling point and boiling range | No data available |
| g) Flash point                             | No data available |
| h) Evaporation rate                        | No data available |
| i) Flammability (solid, gas)               | No data available |
| j) Upper/lower                             | No data available |

flammability or  
explosive limits

- |                                           |                   |
|-------------------------------------------|-------------------|
| k) Vapour pressure                        | No data available |
| l) Vapour density                         | No data available |
| m) Relative density                       | No data available |
| n) Water solubility                       | No data available |
| o) Partition coefficient: n-octanol/water | log Pow: 8.336    |
| p) Auto-ignition temperature              | No data available |
| q) Decomposition temperature              | No data available |
| r) Viscosity                              | No data available |
| s) Explosive properties                   | No data available |
| t) Oxidizing properties                   | No data available |

## 9.2 Other safety information

No data available

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## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

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

Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

Inhalation: No data available

Dermal: No data available

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.
- ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
- NTP: No component 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 identified as a carcinogen or potential carcinogen by OSHA.

**Reproductive toxicity**

No data available

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

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**12. ECOLOGICAL INFORMATION****12.1 Toxicity**

No data available

**12.2 Persistence and degradability**

No data available

**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 Other adverse effects**

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

No data available

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**13. DISPOSAL CONSIDERATIONS****13.1 Waste treatment methods****Product**

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

**Contaminated packaging**

Dispose of as unused product.

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**14. TRANSPORT INFORMATION****DOT (US)**

Not dangerous goods

**IMDG**

Not dangerous goods

**IATA**

Not dangerous goods

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**15. REGULATORY INFORMATION****SARA 302 Components**

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

**SARA 313 Components**

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 311/312 Hazards**

No SARA Hazards

**Massachusetts Right To Know Components**

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

**Pennsylvania Right To Know Components**

XCT790

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725247-18-7

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**New Jersey Right To Know Components**

XCT790

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**California Prop. 65 Components**

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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**16. OTHER INFORMATION****Full text of H-Statements referred to under sections 2 and 3.**

H413 May cause long lasting harmful effects to aquatic life.

**HMIS Rating**

|                        |   |
|------------------------|---|
| Health hazard:         | 0 |
| Chronic Health Hazard: |   |
| Flammability:          | 0 |
| Physical Hazard        | 0 |

**NFPA Rating**

|                    |   |
|--------------------|---|
| Health hazard:     | 0 |
| Fire Hazard:       | 0 |
| Reactivity Hazard: | 0 |

**Further information**

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**Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

Version: 3.6

Revision Date: 09/29/2017

Print Date: 11/10/2018