

SAFETY DATA SHEET

Version 6.1
Revision Date 05/28/2017
Print Date 10/04/2019

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : LY225910

Product Number : L2545

Brand : Sigma

CAS-No. : 133040-77-4

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 Inc.
3050 Spruce Street
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 3), H301

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



Signal word

Danger

Hazard statement(s)

H301

Toxic if swallowed.

H413

May cause long lasting harmful effects to aquatic life.

Precautionary statement(s)

P264

Wash skin thoroughly after handling.

P270

Do not eat, drink or smoke when using this product.

P273

Avoid release to the environment.

P301 + P310

IF SWALLOWED: Immediately call a POISON CENTER/doctor.

P321

Specific treatment (see supplemental first aid instructions on this label).

P330	Rinse mouth.
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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : 2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone

Formula : C₂₇H₂₄BrN₃O₂

Molecular weight : 502.40 g/mol

CAS-No. : 133040-77-4

Hazardous components

Component	Classification	Concentration
2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone		
	Acute Tox. 3; Aquatic Chronic 4; H301, H413	<= 100 %

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

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. Move out of dangerous area.

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. Take victim immediately to hospital. 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

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

Carbon oxides, Nitrogen oxides (NO_x), Hydrogen bromide gas

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. 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.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. 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

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

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection

Face shield and safety glasses 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

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use (EN 143) respirator cartridges as a backup to engineering controls. If th full-face supplied air respirator. 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.

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	179 - 181 °C (354 - 358 °F)
f) Initial boiling point and boiling range	625.3 - 755.30 °C (1157.5 - 1391.54 °F) at 1,013.25 hPa
g) Flash point	337 - 405.6 °C (639 - 762.1 °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) Vapour pressure	No data available
l) Vapour density	No data available
m) Relative density	1.38 - 1.40 g/cm ³
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	log Pow: 6.942
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

Dissociation constant	15.9 - 16.5 at 25 °C (77 °F) 1.65 - 3.05 at 25 °C(77 °F)
-----------------------	---

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

Other decomposition products - No data available

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Hydrogen bromide gas

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

No data available(2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone

Inhalation: No data available(2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone)

Dermal: No data available(2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone)

No data available(2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone)

Skin corrosion/irritation

Serious eye damage/eye irritation

No data available(2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone)

Respiratory or skin sensitisation

No data available(2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone)

Germ cell mutagenicity

No data available(2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone)

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(2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone)

No data available(2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone)

Specific target organ toxicity - single exposure

No data available(2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone)

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available(2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone)

Additional Information

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.(2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone)

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 (2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone)

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

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chem scrubber.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 2811 Class: 6.1

Packing group: III

Proper shipping name: Toxic solids, organic, n.o.s. (2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone)

Poison Inhalation Hazard: No

IMDG

UN number: 2811 Class: 6.1

Packing group: III

EMS-No: F-A, S-A

Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone)

IATA

UN number: 2811 Class: 6.1

Packing group: III

Proper shipping name: Toxic solid, organic, n.o.s. (2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4-(3H)-quinazolinone)

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

Acute Health Hazard

Massachusetts Right To Know Components

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

Pennsylvania Right To Know Components

2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)
phenyl]-4-(3H)-quinazolinone

CAS-No.
133040-77-4

Revision Date

New Jersey Right To Know Components

2-[2-(5-Bromo-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)
phenyl]-4-(3H)-quinazolinone

CAS-No.
133040-77-4

Revision Date

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.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

H301 Toxic if swallowed.
H413 May cause long lasting harmful effects to aquatic life.

HMIS Rating

Health hazard: 2
Chronic Health Hazard:
Flammability: 1
Physical Hazard 0

NFPA Rating

Health hazard: 2
Fire Hazard: 1
Reactivity Hazard: 0

Further information

Copyright 2016 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956
Version: 6.1

Revision Date: 05/28/2017

Print Date: 10/04/2019