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1 Identification

- · Product identifier
- Trade name: SARS-CoV-2 main Protease Inhibitor
- Article number: 701964
- · Application of the substance / the mixture For research use only, not for human or veterinary use.

· Details of the supplier of the safety data sheet

Manufacturer/Supplier: Cayman Chemical Co. 1180 E. Ellsworth Rd. Ann Arbor, MI 48108 USA

- · Information department: Product safety department
- Emergency telephone number: During normal opening times: +1 (734) 971-3335 US/CANADA: 800-424-9300 Outside US/CANADA: 703-741-5970

2 Hazard(s) identification

· Classification of the substance or mixture

Flam. Liq. 4 H227 Combustible liquid.

- · Label elements
- · GHS label elements
- The product is classified and labeled according to the Globally Harmonized System (GHS).
- Hazard pictograms None
- · Signal word Warning
- · Hazard statements

H227 Combustible liquid.

- Precautionary statements
- P210 Keep away from flames and hot surfaces. No smoking.
- P280 Wear protective gloves/protective clothing/eye protection/face protection.

P370+P378 In case of fire: Use CO2, powder or water spray to extinguish.

- P403+P235 Store in a well-ventilated place. Keep cool.
- P501 Dispose of contents/container in accordance with local/regional/national/international regulations.
- · Classification system:
- NFPA ratings (scale 0 4)

Health = 0 Fire = 1 Reactivity = 0

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99.75%

0.25%

· HMIS-ratings (scale 0 - 4)



Reactivity = 0

· Other hazards

· Results of PBT and vPvB assessment

· **PBT:** Not applicable.

· vPvB: Not applicable.

3 Composition/information on ingredients

· Chemical characterization: Mixtures

• **Description:** Mixture of the substances listed below with nonhazardous additions.

· Dangerous components:

CAS: 67-68-5 Dimethyl sulfoxide, anhydrous

RTECS: PV6210000

· Other ingredients

1416992-39-6 GC376 (sodium salt)

4 First-aid measures

· Description of first aid measures

· After inhalation: Supply fresh air; consult doctor in case of complaints.

• After skin contact: Generally the product does not irritate the skin.

- After eye contact: Rinse opened eye for several minutes under running water.
- · After swallowing: If symptoms persist consult doctor.

· Information for doctor:

- · Most important symptoms and effects, both acute and delayed May cause anemia, cough, CNS depression, drowsiness, headache, heart damage, lassitude (weakness, exhaustion), liver damage, narcosis, reproductive effects, teratogenic effects. No further relevant information available.
- · Indication of any immediate medical attention and special treatment needed No further relevant information available.

5 Fire-fighting measures

- · Extinguishing media
- · Suitable extinguishing agents: CO2, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam. Special hazards arising from the substance or mixture Can release vapors that form explosive mixtures at temperatures at or above the flashpoint. Container explosion may occur under fire conditions. Emits toxic fumes under fire conditions. Sensitive to static discharge. Vapors can travel to a source of ignition and flash back.

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· Advice for firefighters

• Protective equipment: No special measures required.

6 Accidental release measures

- Personal precautions, protective equipment and emergency procedures
 Wear protective equipment. Keep unprotected persons away.
 Environmental precautions:
- Dilute with plenty of water.

Do not allow to enter sewers/ surface or ground water.

- Methods and material for containment and cleaning up: Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust). Dispose contaminated material as waste according to item 13. Ensure adequate ventilation.
 Reference to other sections
- See Section 7 for information on safe handling. See Section 8 for information on personal protection equipment. See Section 13 for disposal information. • Protective Action Criteria for Chemicals

· PAC-1:	
67-68-5 Dimethyl sulfoxide, anhydrous	150 ppm
· PAC-2:	
67-68-5 Dimethyl sulfoxide, anhydrous	290 ppm
· PAC-3:	
67-68-5 Dimethyl sulfoxide, anhydrous	1,800 ppm

7 Handling and storage

· Handling:

- Precautions for safe handling
- No special precautions are necessary if used correctly. Avoid breathing dust/fume/gas/mist/vapours/spray. Avoid prolonged or repeated exposure. Keep away from sources of ignition. Take precautionary measures against static discharge.re.
- Information about protection against explosions and fires: Keep ignition sources away - Do not smoke.
- Conditions for safe storage, including any incompatibilities Keep container tightly closed.
 Store in accordance with information listed on the product insert.
 Storage:
- Requirements to be met by storerooms and receptacles: No special requirements.
- Information about storage in one common storage facility: Not required.
- Further information about storage conditions: Keep receptacle tightly sealed.
- · Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

· Additional information about design of technical systems: No further data; see item 7.

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Control parameters

• Components with limit values that require monitoring at the workplace:

67-68-5 Dimethyl sulfoxide, anhydrous

WEEL Long-term value: 250 ppm

· Additional information: The lists that were valid during the creation were used as basis.

· Exposure controls

- · Personal protective equipment:
- · General protective and hygienic measures: Wash hands before breaks and at the end of work.
- Breathing equipment: Not required.
- Protection of hands:



Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation. Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

• Material of gloves

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer. As the product is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.

Penetration time of glove material

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

• Eye protection: Goggles recommended during refilling.

Information on basic physical and General Information	chemical properties	
Appearance:		
Form:	Liquid	
Color:	According to product specification	
Odor:	Characteristic	
Structural Formula	C H3 S O - C H3	
Molecular Weight	78.1 g/mol	
Odor threshold:	Not determined.	
pH-value:	Not determined.	
Change in condition		
Melting point/Melting range:	18.45 °C (65.2 °F)	
Boiling point/Boiling range:	189 °C (372.2 °F)	
Flash point:	95 °C (203 °F)	
Flammability (solid, gaseous):	Not applicable.	
Ignition temperature:	270 °C (518 °F)	

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Decomposition temperature:	Not determined.	
Auto igniting:	Product is not selfigniting.	
Danger of explosion:	Not determined.	
Explosion limits:		
Lower:	1.8 Vol %	
Upper:	63 Vol %	
Vapor pressure at 20 °C (68 °F):	2.5 hPa (1.9 mm Hg)	
Density at 20 °C (68 °F):	1.1 g/cm³ (9.1795 lbs/gal)	
Relative density	Not determined.	
Vapor density	Not determined.	
Evaporation rate	Not determined.	
Solubility in / Miscibility with		
Water:	Fully miscible.	
Partition coefficient (n-octanol/w	ater): Not determined.	
Viscosity:		
Dynamic at 20 °C (68 °F):	198 mPas	
Kinematic:	Not determined.	
Solvent content:		
Organic solvents:	99.8 %	
VOC content:	99.75 %	
	1,097.3 g/l / 9.16 lb/gal	
Solids content:	1.0 %	
Other information	No further relevant information available.	

10 Stability and reactivity

· Reactivity No further relevant information available.

- · Chemical stability
- Thermal decomposition / conditions to be avoided:

No decomposition if used according to specifications.

- Possibility of hazardous reactions No dangerous reactions known.
- · Conditions to avoid No further relevant information available.
- · Incompatible materials: No further relevant information available.
- · Hazardous decomposition products: No dangerous decomposition products known.

11 Toxicological information

· Information on toxicological effects

• Acute toxicity:

· LD/LC50 values that are relevant for classification:

67-68-5 Dimethyl sulfoxide, anhydrous

Oral LD50 14,500 mg/kg (rat)

Primary irritant effect:

• on the skin: No irritant effect.

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- on the eye: No irritating effect.
- Sensitization: No sensitizing effects known.
- Additional toxicological information:

· Carcinogenic categories

· IARC (International Agency for Research on Cancer)

None of the ingredients is listed.

· NTP (National Toxicology Program)

None of the ingredients is listed.

· OSHA-Ca (Occupational Safety & Health Administration)

None of the ingredients is listed.

12 Ecological information

- · Toxicity
- Aquatic toxicity: No further relevant information available.
- **Persistence and degradability** No further relevant information available.
- · Behavior in environmental systems:
- · Bioaccumulative potential No further relevant information available.
- Mobility in soil No further relevant information available.
- · Additional ecological information:
- · General notes:
- Water hazard class 1 (Self-assessment): slightly hazardous for water

Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

- Results of PBT and vPvB assessment
- **PBT:** Not applicable.
- **vPvB:** Not applicable.
- Other adverse effects No further relevant information available.

13 Disposal considerations

- · Waste treatment methods
- · Recommendation:

Must not be disposed of together with household garbage. Do not allow product to reach sewage system.

- · Uncleaned packagings:
- Recommendation: Disposal must be made according to official regulations.
- · Recommended cleansing agent: Water, if necessary with cleansing agents.

· UN-Number		
DOT, IMDG, IATA	UN1993	
UN proper shipping name		
DOT	Flammable liquids, n.o.s.	
·IMDG	FLAMMABLE LIQUID, N.O.S.	

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	Flammable liquid, n.o.s.
· Transport hazard class(es)	
DOT	
RAMARE LOUD	
3	
Class	3 Flammable liquids
· Label	3
· IMDG, IATA	
Class	3 Flammable liquids
Label	3
 Packing group DOT, IMDG, IATA 	
Environmental hazards:	Not applicable.
· Special precautions for user	Warning: Flammable liquids
Hazard identification number (Kemler code):	
· EMS Number: · Stowage Category	F-E, <u>S-E</u> A
• Transport in bulk according to Annex II of	· ·
MARPOL73/78 and the IBC Code	Not applicable.
· Transport/Additional information:	
DOT	
Quantity limitations	On passenger aircraft/rail: 60 L
INDO	On cargo aircraft only: 220 L
· IMDG · Limited quantities (LQ)	5L
Excepted quantities (EQ)	Code: E1
	Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 1000 ml
IATA	
· Remarks:	When sold in quantities of less than or equal to 1 ml
	or 1 g, with an Excepted Quantity Code of
	E1, E2, E4, or E5, this item meets the De Minimi Quantities exemption, per IATA 2.6.10.
	Therefore packaging does not have to be labeled a
	Dangerous Goods/Excepted Quantity.
· UN "Model Regulation":	UN 1993 FLAMMABLE LIQUID, N.O.S., 3, III

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	latory information
	, health and environmental regulations/legislation specific for the substance or mixture
No furt • Sara	her relevant information available.
	n 355 (extremely hazardous substances):
	of the ingredients is listed.
- Sectio	n 313 (Specific toxic chemical listings):
	of the ingredients is listed.
· TSCA	(Toxic Substances Control Act):
67-68-	5 Dimethyl sulfoxide, anhydrous ACTIVE
· Hazaro	dous Air Pollutants
None of	of the ingredients is listed.
· Propo	sition 65
[.] Chemi	icals known to cause cancer:
None o	of the ingredients is listed.
· Chemi	cals known to cause reproductive toxicity for females:
None of	of the ingredients is listed.
[.] Chemi	cals known to cause reproductive toxicity for males:
None of	of the ingredients is listed.
· Chemi	cals known to cause developmental toxicity:
None of	of the ingredients is listed.
· Carcin	logenic categories
· EPA (E	Environmental Protection Agency)
None of	of the ingredients is listed.
· TLV (T	hreshold Limit Value)
None of	of the ingredients is listed.
· NIOSH	I-Ca (National Institute for Occupational Safety and Health)
None of	of the ingredients is listed.
	ical safety assessment: A Chemical Safety Assessment has not been carried out

• Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information

All chemicals may pose unknown hazards and should be used with caution. This SDS applies only to the material as packaged. If this product is combined with other materials, deteriorates, or becomes contaminated, it may pose hazards not mentioned in this SDS. Cayman Chemical Company assumes no responsibility for incidental or consequential damages, including lost profits, arising from the use of these data. It shall be the user's responsibility to develop proper methods of handling and personal protection based on the actual conditions of use. While this SDS is based on technical data judged to be reliable, Cayman Chemical Company assumes no responsibility for the completeness or accuracy of the information contained herein.

- · Department issuing SDS: Environment protection department.
- · Contact: -
- · Date of preparation / last revision 08/07/2021 / -
- Abbreviations and acronyms: IMDG: International Maritime Code for Dangerous Goods DOT: US Department of Transportation

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IATA: International Air Transport Association	· · · · · · ·
EINECS: European Inventory of Existing Commercial Chemical Substances	
ELINCS: European List of Notified Chemical Substances	
CAS: Chemical Abstracts Service (division of the American Chemical Society)	
NFPA: National Fire Protection Association (USA)	
HMIS: Hazardous Materials Identification System (USA)	
VOC: Volatile Organic Compounds (USA, ÉU)	
LC50: Lethal concentration, 50 percent	
LD50: Lethal dose, 50 percent	
PBT: Persistent, Bioaccumulative and Toxic	
vPvB: very Persistent and very Bioaccumulative	
NIOSH: National Institute for Occupational Safety	
OSHA: Occupational Safety & Health	
TLV: Threshold Limit Value	
PEL: Permissible Exposure Limit	
REL: Recommended Exposure Limit	
Flam. Lig. 4: Flammable liquids – Category 4	
* Data compared to the previous version altered.	
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