Safety Data Sheet
acc. to OSHA HCS

Printing date 08/26/2024 Revision date 08/26/2024

*

1 Identification

· **Product identifier**

· **Trade name: Pyrrophenone**
· **Synonym**
N-[[(2S,4R)-1-[2-(2,4-difluorobenzoyl)benzoyl]-4-[(triphenylmethyl)thio]-2-pyrrolidinyl]methyl]-4-[(Z)-(2,4-dioxo-5-thiazolidinylidene)methyl]-benzamide

· **Article number:** 13294
· **CAS Number:**
341973-06-6
· **Application of the substance / the mixture**
This product is for research use - Not for human or veterinary diagnostic or therapeutic use.

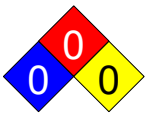
· **Details of the supplier of the safety data sheet**
· **Manufacturer/Supplier:**
Cayman Chemical Co.
1180 E. Ellsworth Rd.
Ann Arbor, MI 48108
USA

· **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**
The substance is not classified, according to the Globally Harmonized System (GHS).

· **Label elements**
· **GHS label elements** None
· **Hazard pictograms** None
· **Signal word** None
· **Hazard statements** None
· **Classification system:**
· **NFPA ratings (scale 0 - 4)**



Health = 0
Fire = 0
Reactivity = 0

· **HMIS-ratings (scale 0 - 4)**

Health = 0
Fire = 0
Reactivity = 0

(Contd. on page 2)

Safety Data Sheet
acc. to OSHA HCS

Printing date 08/26/2024 Revision date 08/26/2024

Trade name: Pyrrophenone

(Contd. from page 1)

· **Other hazards**
· **Results of PBT and vPvB assessment**
· **PBT:** Not applicable.
· **vPvB:** Not applicable.

3 Composition/information on ingredients

· **Chemical characterization: Substances**
· **CAS No. Description**
341973-06-6 Pyrrophenone

4 First-aid measures

· **Description of first aid measures**
· **General information:** No special measures required.
· **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**
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:**
Use fire fighting measures that suit the environment.
A solid water stream may be inefficient.
· **Special hazards arising from the substance or mixture** No further relevant information available.
· **Advice for firefighters**
· **Protective equipment:** No special measures required.

6 Accidental release measures

· **Personal precautions, protective equipment and emergency procedures** Not required.
· **Environmental precautions:** 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).
· **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:** Substance is not listed.
· **PAC-2:** Substance is not listed.

(Contd. on page 3)

Safety Data Sheet
acc. to OSHA HCS

Printing date 08/26/2024 Revision date 08/26/2024

Trade name: Pyrrophenone

(Contd. from page 2)

· **PAC-3:** Substance is not listed.

7 Handling and storage

· **Handling:**
· **Precautions for safe handling** No special measures required.
· **Information about protection against explosions and fires:** No special measures required.

· **Conditions for safe storage, including any incompatibilities**
· **Storage:** Store in accordance with information listed on the product insert.
· **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:** None.
· **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 section 7.

· **Control parameters**
· **Components with limit values that require monitoring at the workplace:** Not required.
· **Additional information:** The lists that were valid during the creation were used as basis.

· **Exposure controls**
· **Personal protective equipment:**
· **General protective and hygienic measures:**
The usual precautionary measures for handling chemicals should be followed.
· **Breathing equipment:** Not required.
· **Protection of hands:**
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.
· **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.

9 Physical and chemical properties

· **Information on basic physical and chemical properties**
· **General Information**
· **Appearance:**

Form:	Solid
Color:	Not determined.
· **Odor:**	Characteristic
· **Structural Formula**	C49H37F2N3O5S2
· **Molecular Weight**	850 g/mol

(Contd. on page 4)

Safety Data Sheet
acc. to OSHA HCS

Printing date 08/26/2024 Revision date 08/26/2024

Trade name: Pyrrophenone

(Contd. from page 3)

· **Odor threshold:**	Not determined.
· **pH-value:**	Not determined.
· **Change in condition**	
Melting point/Melting range:	Undetermined.
Boiling point/Boiling range:	Undetermined.
· **Flash point:**	Not applicable.
· **Flammability:**	Not applicable.
· **Decomposition temperature:**	Not determined.
· **Ignition temperature:**	Not determined.
· **Danger of explosion:**	Product does not present an explosion hazard.
· **Explosion limits:**	
Lower:	Not determined.
Upper:	Not determined.
· **Vapor pressure:**	Not determined.
· **Density:**	Not determined.
· **Relative density**	Not determined.
· **Vapor density**	Not determined.
· **Evaporation rate**	Not determined.
· **Solubility in / Miscibility with**	
Water:	Not determined.
· **Partition coefficient (n-octanol/water):**	Not determined.
· **Viscosity:**	
Dynamic:	Not determined.
Kinematic:	Not determined.
SOLUBILITY	DMF: 12.5 mg/ml; DMSO: 15 mg/ml; DMSO:PBS (pH 7.2) (1:10): 0.1 mg/ml
· **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:** strong oxidizing agents
· **Hazardous decomposition products:** carbon dioxide, carbon monoxide, hydrogen fluoride

(Contd. on page 5)

Safety Data Sheet
acc. to OSHA HCS

Printing date 08/26/2024 Revision date 08/26/2024

Trade name: Pyrrophenone

(Contd. from page 4)

11 Toxicological information

· **Information on toxicological effects**
· **Acute toxicity:**
· **Primary irritant effect:**
· **on the skin:** No irritant effect.
· **on the eye:** No irritating effect.
· **Sensitization:** No sensitizing effects known.
· **Additional toxicological information:**
When used and handled according to specifications, the product does not have any harmful effects according to our experience and the information provided to us.
The substance is not subject to classification.

· **Carcinogenic categories**
· **IARC (International Agency for Research on Cancer)** Substance is not listed.
· **NTP (National Toxicology Program)** Substance is not listed.
· **OSHA-Ca (Occupational Safety & Health Administration)** Substance is not 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:** Smaller quantities can be disposed of with household waste.

· **Uncleaned packagings:**
· **Recommendation:** Disposal must be made according to official regulations.

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14 Transport information

· **UN-Number**
· **DOT, IMDG, IATA** not regulated

(Contd. on page 6)

Safety Data Sheet
acc. to OSHA HCS

Printing date 08/26/2024 Revision date 08/26/2024

Trade name: Pyrrophenone

(Contd. from page 5)

· **UN proper shipping name** · **DOT, IMDG, IATA**	not regulated
· **Transport hazard class(es)** · **DOT, ADN, IMDG, IATA** · **Class**	not regulated
· **Packing group** · **DOT, IMDG, IATA**	not regulated
· **Environmental hazards:**	Not applicable.
· **Special precautions for user**	Not applicable.
· **Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code**	Not applicable.
· **UN "Model Regulation":**	not regulated

15 Regulatory information

· **Safety, health and environmental regulations/legislation specific for the substance or mixture**
No further relevant information available.
· **Sara**
· **Section 355 (extremely hazardous substances):** Substance is not listed.
· **Section 313 (Specific toxic chemical listings):** Substance is not listed.
· **TSCA (Toxic Substances Control Act):** Substance is not listed.
· **Hazardous Air Pollutants** Substance is not listed.
· **Proposition 65**
· **Chemicals known to cause cancer:** Substance is not listed.
· **Chemicals known to cause reproductive toxicity for females:** Substance is not listed.
· **Chemicals known to cause reproductive toxicity for males:** Substance is not listed.
· **Chemicals known to cause developmental toxicity:** Substance is not listed.

· **Carcinogenic categories**
· **EPA (Environmental Protection Agency)** Substance is not listed.
· **TLV (Threshold Limit Value)** Substance is not listed.
· **NIOSH-Ca (National Institute for Occupational Safety and Health)** Substance is not listed.
· **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** 08/26/2024 / -

(Contd. on page 7)

Safety Data Sheet
acc. to OSHA HCS

Printing date 08/26/2024 Revision date 08/26/2024

Trade name: Pyrrophenone

(Contd. from page 6)

· **Abbreviations and acronyms:**
IMDG: International Maritime Code for Dangerous Goods
DOT: US Department of Transportation
IATA: International Air Transport Association
CAS: Chemical Abstracts Service (division of the American Chemical Society)
NFPA: National Fire Protection Association (USA)
HMIS: Hazardous Materials Identification System (USA)
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

· *** Data compared to the previous version altered.**