

SAFETY DATA SHEET

Creation Date 15-Jul-2014

Revision Date 18-Dec-2025

Revision Number 6

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

1. Identification

Product Name Caffeine

Cat No. : AC108160000; AC108160025; AC108160050; AC108160100;
AC108165000

CAS No 58-08-2
Synonyms 3,7-Dihydro-1,3,7-trimethyl-1H-purine-2,6-dione

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11

Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99

CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

This chemical is considered hazardous according to [US] OSHA (29 CFR 1910.1200, 2024)

Acute oral toxicity

Category 4

Label Elements

Signal Word

Warning

Hazard Statements

Harmful if swallowed

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product

Ingestion

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
Rinse mouth

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

Hazards classified under paragraph (d)(1)(ii) of 1910.1200

No information available

3. Composition/information on Ingredients

Component	CAS No	Weight %
Caffeine	58-08-2	<=100

4. First-aid measures

General Advice	If symptoms persist, call a physician.
Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Ingestion	Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.
Most important symptoms and effects	None reasonably foreseeable.
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray, carbon dioxide (CO ₂), dry chemical, alcohol-resistant foam.
Unsuitable Extinguishing Media	No information available
Flash Point	No information available
Method -	No information available

Autoignition Temperature 540 °C / 1004 °F

Explosion Limits

Upper No data available
Lower No data available
Sensitivity to Mechanical Impact No information available
Sensitivity to Static Discharge No information available

Specific Hazards Arising from the Chemical

Thermal decomposition can lead to release of irritating gases and vapors. Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NO_x).

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health
2

Flammability
1

Instability
0

Physical hazards
N/A

6. Accidental release measures

Personal Precautions Use personal protective equipment as required. Ensure adequate ventilation. Avoid dust formation.

Environmental Precautions Should not be released into the environment.

Methods for Containment and Clean Up Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

7. Handling and Storage

Handling Wear personal protective equipment/face protection. Ensure adequate ventilation. Avoid dust formation. Avoid ingestion and inhalation. Do not get in eyes, on skin, or on clothing.

Storage. Keep containers tightly closed in a dry, cool and well-ventilated place. Incompatible Materials. Strong oxidizing agents.

8. Exposure controls / personal protection

Exposure Guidelines This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

Engineering Measures Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal Protective Equipment

Eye/face Protection Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended Filter type:	Particulates filter conforming to EN 143.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Appearance

Physical State	Solid		
Color	White		
Odor	Odorless		
Odor Threshold	No information available		
Property	Values	Remarks	• Method
Melting Point/Range	234 - 239 °C / 453.2 - 462.2 °F		
Softening Point	No data available		
Boiling Point/Range	No information available		
Flash Point	No information available	Method -	No information available
Flammability (liquid)	Not applicable	Solid	
Flammability (solid,gas)	No information available		
Explosion Limits	No data available		
Autoignition Temperature	540 °C / 1004 °F		
Decomposition Temperature	No data available		
pH	5.5-6.5	20 g/L (20°C)	
Viscosity	Not applicable	Solid	
Water Solubility	20g/L (20°C)		
Solubility in other solvents	No information available		
Partition Coefficient (n-octanol/water)			
Component	log Pow		
Caffeine	-0.091		
Vapor Pressure	15 mmHg @ 89 °C		
Density / Specific Gravity	1.230		
Bulk Density	No data available		
Vapor Density	Not applicable	Solid	
Particle characteristics	No data available		
Other Information			
Molecular Formula	C8 H10 N4 O2		
Molecular Weight	194.19		
Evaporation Rate	Not applicable - Solid		

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	Avoid dust formation. Incompatible products. Excess heat.
Incompatible Materials	Strong oxidizing agents
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂), Nitrogen oxides (NO _x)
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Information on expected route of exposure

Inhalation	Not an expected route of exposure.
Ingestion	May be harmful if swallowed.
Eyes	Avoid contact with eyes.
Skin	Avoid contact with skin.

Toxicology data for the components

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Caffeine	LD50 = 367.7 mg/kg (Rat)	LD50 > 2000 mg/kg (Rat)	LC50 = 4.94 mg/L (Rat) 4 h

Toxicologically Synergistic Products No information available

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;
Respiratory No data available
Skin No data available

(e) germ cell mutagenicity; No data available
 Not mutagenic in AMES Test

(f) carcinogenicity;

The table below indicates whether each agency has listed any ingredient as a carcinogen

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Caffeine	58-08-2	Not listed	Not listed	Not listed	Not listed	Not listed

(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available
Target Organs None known.

(j) aspiration hazard; Not applicable
 Solid

Symptoms / effects, both acute and delayed No information available.

Other Adverse Effects The toxicological properties have not been fully investigated.

Endocrine Disrupting Properties This product does not contain any known or suspected endocrine disruptors.

12. Ecological information

Ecotoxicity

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Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Caffeine	Not listed	LC50: = 151 mg/L, 96h flow-through (Pimephales promelas)	Not listed	Not listed

Persistence and Degradability Persistence is unlikely

Bioaccumulation/ Accumulation No information available.

Mobility . Will likely be mobile in the environment due to its water solubility.

Component	log Pow
Caffeine	-0.091

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT Not regulated
TDG Not regulated
IATA Not regulated
IMDG/IMO Not regulated

15. Regulatory Information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Caffeine	58-08-2	X	ACTIVE	-

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT)

Not applicable

TSCA 12(b) - Notices of Export

Not applicable

International Inventories

China, X = listed, Australia, U.S.A. (TSCA), Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Australia (AICS), Korea (KECL), China (IECSC), Japan (ENCS), Philippines (PICCS), Taiwan (TCSI), Japan (ISHL), New Zealand (NZIoC), Japan (ISHL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Caffeine	58-08-2	X	-	200-362-1	X	X	X	X	X	KE-10766

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

U.S. Federal Regulations

SARA 313

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations Not applicable

U.S. Department of Transportation

Reportable Quantity (RQ): N

DOT Marine Pollutant N

DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Caffeine	58-08-2	-	-	-

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

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Caffeine	58-08-2	Listed	Not applicable	Not applicable	Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Other International Regulations

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Caffeine	58-08-2	Not applicable	Not applicable	Not applicable	Not applicable

16. Other Information

Prepared By	Product stewardship (Regulatory Affairs) Thermo Fisher Scientific email - begel.sdsdesk@thermofisher.com
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Revision Summary	Updated to the U.S. Department of Labor's Occupational Safety and Health Administration (OSHA) which published its Final Rule in the Federal Register revising the Hazard Communication Standard (HCS/HazCom), 29 CFR 1910.1200 (2024) (HCS §1910.1200, 2024), May 20, 2024, effective July 19, 2024.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS