

Safety Data Sheet

AICAR · Acadesine · CAS 2627-69-2

Issued by
Calibre Labs LLC
trading as Pure Peptides

Prepared to
OSHA HazCom 2012
29 CFR 1910.1200 / GHS

Version
1.0
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Section 1 — Identification

Product identifier: AICAR

Synonyms: Acadesine; AICAR; AICA riboside

CAS number: 2627-69-2

Product code / catalogue: purepeptides.com/product/aicar

Recommended use: In-vitro laboratory research use only. Supplied as a chemical reagent for use by qualified personnel in a controlled laboratory setting.

Uses advised against: Not for human or veterinary use. Not for use as a drug, food, food additive, dietary supplement, or cosmetic ingredient. Not for administration to humans or animals by any route. Not for household or general consumer use.

Supplier:

Calibre Labs LLC, trading as Pure Peptides

1309 Coffeen Avenue STE 20165

Sheridan, WY 82801

United States

team@purepeptides.com

Emergency telephone — medical (human exposure or poisoning):

Poison Help, national Poison Control: **1-800-222-1222**

Available 24 hours a day from anywhere in the United States. Free and confidential. Calls are answered by a trained nurse, pharmacist, or physician at the caller's regional poison center.

Product and chemical enquiries (non-emergency): team@purepeptides.com, business hours.

Section 2 — Hazard(s) identification

GHS classification: Not classified.

This substance has not been assigned a GHS hazard classification. No harmonised classification exists for it, and the toxicological data required to classify it under 29 CFR 1910.1200 Appendix A are not available.

Signal word: None.

Hazard pictograms: None.

Hazard statements: None assigned.

Precautionary statements:

- Avoid generating dust when handling the lyophilized solid.
- Wash hands thoroughly after handling.
- Wear protective gloves, eye protection, and a laboratory coat.

- Do not release to drains or surface water (see Sections 12 and 13).
- Keep container tightly closed and store as specified in Section 7.

Hazards not otherwise classified: None identified.

Important qualification. The absence of a classification is a statement about the available evidence, not a determination that this substance is non-hazardous. This material has not been subjected to toxicological testing. Treat it as a substance of unknown toxicity and handle it under the general precautions for research chemicals set out in Sections 7 and 8.

Section 3 — Composition / information on ingredients

Single-substance material.

Component	Identifier	Concentration
AICAR	CAS 2627-69-2	See batch Certificate of Analysis

Molecular formula: $C_9H_{14}N_4O_5$

Molecular weight: 258.23 g/mol

Composition note. Purity is reported as HPLC area percent, which is a chromatographic measure and not peptide content by weight. The accompanying counter-ion — commonly trifluoroacetate or acetate — and residual water are present in the vial but are not represented in the formula above. The mass in the vial is therefore not entirely the named compound. Batch-specific composition is given on the Certificate of Analysis for the lot supplied.

Section 4 — First-aid measures

In any exposure incident, call Poison Help on 1-800-222-1222 — 24 hours, free, answered by a trained clinician. Have this Safety Data Sheet to hand when you call.

Inhalation. Move the affected person to fresh air and keep them at rest in a position comfortable for breathing. Seek medical attention if symptoms develop or persist.

Skin contact. Remove contaminated clothing. Wash the affected area with soap and water. Seek medical attention if irritation develops or persists.

Eye contact. Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do, then continue rinsing. Seek medical attention if irritation persists.

Ingestion. Rinse the mouth with water. Do not induce vomiting. Do not give anything by mouth to an unconscious person. Seek medical attention.

Most important symptoms and effects: No data available. No symptoms specific to this substance have been characterised.

Indication of immediate medical attention and special treatment: No specific antidote is known. Treat symptomatically. Show this Safety Data Sheet to the attending physician. Note for clinicians: no toxicological data exist for this substance (Section 11).

Section 5 — Fire-fighting measures

Suitable extinguishing media: Water spray, carbon dioxide, dry chemical powder, or alcohol-resistant foam. Select media appropriate to the surrounding fire.

Unsuitable extinguishing media: None known.

Specific hazards arising from the substance: Combustion may produce carbon monoxide, carbon dioxide, and nitrogen oxides.

Special protective equipment for firefighters: Self-contained breathing apparatus and full protective clothing.

Section 6 — Accidental release measures

Personal precautions. Avoid generating airborne dust. Wear the protective equipment specified in Section 8. Restrict access to the affected area until cleanup is complete.

Environmental precautions. Do not allow the material to enter drains, surface water, or groundwater. See Section 12.

Methods and materials for containment and cleanup. Collect the solid by careful mechanical means — sweeping or scooping — without raising dust. For a solution spill, absorb with inert absorbent material. Place recovered material in a labelled, closed container for disposal in accordance with Section 13. Decontaminate the affected surface with water and detergent, collecting the rinsate rather than discharging it to drain.

Section 7 — Handling and storage

This section is specific to this compound and is drawn from the verified handling chemistry established for it.

Handling

Handle the lyophilized powder in a manner that minimises dust generation. Weigh in a balance enclosure or ventilated workspace. Avoid contact with skin and eyes. Do not eat, drink, or smoke in the handling area. Wash hands after handling.

Sterile water is a reasonable default, and PBS or an assay buffer are equally suitable, since there is no metal center to compete for. Add diluent slowly down the inside wall of the vial, swirl gently, and let it stand until it clarifies.

Swirling rather than vortexing matters for a different reason here: a small molecule has no chain to unfold, so the concern is complete dissolution, not denaturation.

N-glycosidic bonds in nucleosides are acid-labile, so strongly acidic diluents can hydrolyze the bond into free base and sugar. Keep preparations near neutral pH.

Adsorptive loss is less of a concern here than for a peptide. Small polar molecules can adsorb onto polypropylene and low-protein-binding tubes reduce it, but this molecule is neutral, with no charged side chains and no hydrophobic surface, so it has little to bind with.

Storage

Store the lyophilized solid at -20 degrees C, sealed, desiccated and protected from light, and let a cold vial warm before opening so condensation does not reach the powder.

Once in solution, hold at 2 to 8 degrees C, or aliquot and freeze for longer storage. Freeze-thaw cycling is less damaging here than for a peptide, since there is no conformation to lose, but aliquoting still limits contamination and concentration drift.

Incompatible materials in storage: See Section 10.

Section 8 — Exposure controls / personal protection

Occupational exposure limits. No occupational exposure limits have been established for this substance. There is no OSHA permissible exposure limit, no ACGIH threshold limit value, and no NIOSH recommended exposure limit assigned to it.

Engineering controls. Handle in a well-ventilated area. Weigh and transfer the dry powder in a balance enclosure, fume hood, or equivalent local exhaust ventilation, to control the dust that is the realistic route of exposure for a lyophilized solid. An eyewash station and access to washing facilities should be available in the work area.

Personal protective equipment:

- **Eye protection:** Safety glasses with side shields, or goggles where splashing is foreseeable.
- **Skin protection:** Chemically resistant gloves — nitrile is appropriate for laboratory-scale handling. Laboratory coat. Change gloves on contamination.
- **Respiratory protection:** Not normally required where powder handling is enclosed or ventilated as above. Where dust cannot be controlled by engineering means, use a NIOSH-approved particulate respirator under a compliant respiratory protection

programme.

General hygiene. Because this substance has no toxicological characterisation, minimise exposure by all routes as a matter of course rather than in response to a known hazard.

Section 9 — Physical and chemical properties

Property	Value
Appearance	Lyophilized powder
Physical state	Solid
Odour	No data available
Odour threshold	No data available
pH	No data available
Melting point / freezing point	No data available
Initial boiling point	No data available
Flash point	No data available
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	No data available
Solubility in water	Soluble. No experimental quantitative figure is available.
Partition coefficient (n-octanol/water)	No data available
Auto-ignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Molecular formula	$C_9H_{14}N_4O_5$
Molecular weight	258.23 g/mol

Note on data provenance. Molecular weight is a computed value. No experimentally determined physical property values are available for this substance.

Section 10 — Stability and reactivity

Reactivity: No reactivity hazard is known under normal conditions of handling and storage.

Chemical stability: Stable under the storage conditions specified in Section 7.

Possibility of hazardous reactions: None known.

Conditions to avoid: Elevated temperature, moisture, light, and repeated freeze–thaw cycling of solutions.

Incompatible materials: Strong oxidising agents, strong acids, and strong bases.

Hazardous decomposition products: Carbon monoxide, carbon dioxide, and nitrogen oxides.

Stability note specific to this compound. The weak point is identifiable from the structure. The N-glycosidic bond joining base to sugar is acid-labile and fails first if a solution drifts acidic, hydrolyzing to free 5-aminoimidazole-4-carboxamide and ribose. The carboxamide is a second, more robust liability, since amides hydrolyze under strongly acidic or alkaline conditions. There is no thiol, no ester and no metal-ligand bond, so the routes that dominate peptides and metal complexes do not apply.

Section 11 — Toxicological information

No toxicological data are available for this substance. It has not been tested for the endpoints below.

Endpoint	Data
Acute oral toxicity (LD50)	No data available
Acute dermal toxicity (LD50)	No data available
Acute inhalation toxicity (LC50)	No data available
Skin corrosion / irritation	No data available
Serious eye damage / irritation	No data available
Respiratory or skin sensitisation	No data available
Germ cell mutagenicity	No data available
Carcinogenicity	No data available
Reproductive toxicity	No data available
STOT — single exposure	No data available
STOT — repeated exposure	No data available
Aspiration hazard	No data available

Carcinogen listings: Not listed by NTP, IARC, or OSHA.

Likely routes of exposure: Inhalation of dust, skin contact, eye contact, and accidental ingestion.

Interpretation. No inference of safety should be drawn from the absence of data in this section. These endpoints are unpopulated because the substance has not been studied, not because it has been studied and found negative.

Section 12 — Ecological information

Ecotoxicity: No ecotoxicological data are available for this substance.

Persistence and degradability: No data available.

Bioaccumulative potential: No data available.

Mobility in soil: No data available.

Other adverse effects: No data available.

Practical direction. Do not discharge this material, solutions of it, or rinsate from decontamination to drains, surface water, or groundwater. Route it to chemical waste as set out in Section 13.

Section 13 — Disposal considerations

Dispose of this material and its container as chemical waste in accordance with applicable federal, state, and local regulations. Do not discharge to drains or the environment.

Contaminated packaging should be handled as the material itself unless it has been decontaminated, with the rinsate collected rather than discharged.

Section 14 — Transport information

UN number: Not assigned. Not classified as a dangerous good.

Regulation	Status
US DOT (49 CFR)	Not regulated as a hazardous material
IATA (air)	Not regulated as dangerous goods
IMDG (sea)	Not regulated as dangerous goods

UN proper shipping name: Not applicable.

Transport hazard class: Not applicable.

Packing group: Not applicable.

Environmental hazards — marine pollutant: Not classified as a marine pollutant.

Special precautions for user: Transport in a closed, labelled container. Maintain the storage conditions in Section 7 where product integrity is required.

Section 15 — Regulatory information

Regulation	Status
TSCA (Toxic Substances Control Act)	Supplied under the research and development exemption at 40 CFR 720.36 — small quantities, for non-commercial research and analysis, used under the supervision of a technically qualified individual.
EPCRA Section 302 — extremely hazardous substances	Not listed.
EPCRA Section 313 — toxic chemical release reporting (TRI)	Not listed.
CERCLA — reportable quantity	Not listed. No reportable quantity is assigned.
California Proposition 65	Not listed.
RCRA — hazardous waste	Not a listed hazardous waste (F, K, P, or U). Waste classification remains the generator's determination — see Section 13.

Product-specific regulatory status. This material is supplied for in-vitro laboratory research use only. It is not approved by the FDA for human or veterinary use and is not a drug, food, dietary supplement, or cosmetic product.

Section 16 — Other information

Revision date: 2026-08-28

Version: 1.0

Supersedes: Not applicable — first issue.

Reason for revision: First issue.

Abbreviations used in this document:

ACGIH — American Conference of Governmental Industrial Hygienists · CAS — Chemical Abstracts Service · CERCLA — Comprehensive Environmental Response, Compensation, and Liability Act · DOT — Department of Transportation · EPCRA — Emergency Planning and Community Right-to-Know Act · GHS — Globally Harmonized System of Classification and Labelling of Chemicals · HPLC — high-performance liquid chromatography · IARC — International Agency for Research on Cancer · IATA — International Air Transport Association · IMDG — International Maritime Dangerous Goods · LC50 — median lethal concentration · LD50 — median lethal dose · NIOSH — National Institute for Occupational Safety and Health · NTP — National Toxicology Program · OSHA — Occupational Safety and Health Administration · PEL — permissible exposure limit · RCRA — Resource Conservation and Recovery Act · STOT — specific target organ toxicity · TLV — threshold limit value · TSCA — Toxic Substances Control Act

Disclaimer. This Safety Data Sheet was prepared for a substance supplied for in-vitro laboratory research use only. The information it contains reflects the data available to Pure Peptides at the date of issue. Several sections state that no data are available; this reflects the state of published knowledge for this substance and is not a determination that no hazard exists. The information is provided without warranty, express or implied. Determining that this material is suitable and safe for a particular use, and complying with all applicable law, is the responsibility of the user.