

Safety Data Sheet

N-Acetoxy-2- acetylaminofluorene

Division of Safety
National Institutes
of Health



WARNING!

THIS COMPOUND IS CARCINOGENIC, MUTAGENIC, AND MODERATELY TOXIC. AVOID FORMATION AND BREATHING OF AEROSOLS.

LABORATORY OPERATIONS SHOULD BE CONDUCTED IN A FUME HOOD, GLOVE BOX, OR VENTILATED CABINET.

AVOID SKIN CONTACT: IF EXPOSED, WASH WITH SOAP AND WATER.

FOR EYE EXPOSURE, IRRIGATE IMMEDIATELY WITH LARGE AMOUNTS OF WATER. FOR INGESTION, INDUCE VOMITING. FOR INHALATION, REMOVE VICTIM PROMPTLY TO CLEAN AIR. ADMINISTER RESCUE BREATHING IF NECESSARY. REFER TO PHYSICIAN.

IN CASE OF LABORATORY SPILL, WEAR PROTECTIVE CLOTHING DURING CLEANUP. AVOID SKIN CONTACT OR BREATHING OF AEROSOLS. USE ACETONE TO DISSOLVE COMPOUND. WASH DOWN AREA WITH SOAP AND WATER. DISPOSE OF WASTE SOLUTIONS AND MATERIALS APPROPRIATELY.

A. Background

N-Acetoxy-2-acetylaminofluorene (N-AcO-AAF) has no known use other than for basic research in carcinogenesis, mutagenesis, and DNA repair. It has moderate acute toxicity for rodents, but it is a potent carcinogen at sites of application in rodents. It is strongly mutagenic in in vitro systems.

B. Chemical and Physical Data

1. Chemical Abstract No.: 6098-44-8

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2. Synonyms :

N-AcO-AAF

N-Acetoxy-2-fluorenylacetami

N-Acetoxy-2-acetamidofluorene

N-(Fluoren-2-yl)acetamide

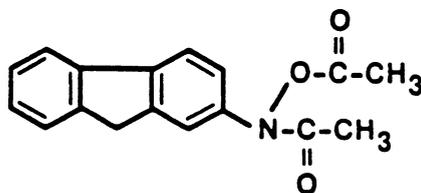
Acetic acid (N-acetyl-N(2-fluorenyl))amino ester

N-(Fluoren-2-yl)acetohydroxamic acetate

N-(Acetyloxy)-N-9H-fluoren-2-yl-acetamide (9CI)

3. Molecular
formula:
C₁₇H₁₅NO₃

structure:



weight:
281.32

4. Density: No data.

5. Absorption spectroscopy: UV: $\lambda = 287$.

6. Volatility: Nonvolatile.

7. Solubility: Slightly soluble in water with decomposition. Soluble in dimethylsulfoxide, acetone, and other organic solvents.

8. Description, appearance: White crystalline solid.

9. Melting point: 112°C (decomposes).

10. Stability: Stable when stored at -20°C as a solid. Decomposes with loss of the acetoxy group and by rearrangement to 1- and 3-acetoxy-2-acetylaminofluorene. Unstable in aqueous solutions. more stable in solvents such as dimethylsulfoxide.

11. Chemical reactivity: The acetoxy group reacts readily with nucleophiles such as methionine, guanosine, and RNA.

12. Flash point: No data.

13. Autoignition temperature: No data.

14. Flammable limits: No data.

Fire, Explosion, and Reactivity Hazard Data

1. N-AcO-AAF does not require special fire-fighting procedures or equipment and does not present unusual fire and explosion hazard.

Because of the electrostatic nature of dry N-AcO-AAF, fire fighters should wear full-face masks.

2. No conditions contributing to instability are known.
3. No incompatibilities have been reported.
4. No hazardous decomposition products are known.
5. N-AcO-AAF does not require nonspark equipment. When handled in organic solvents, the precautions required for such solvents will apply.

Operational Procedures

The NIH Guidelines for the Laboratory Use of Chemical Carcinogens describe operational practices to be followed when potentially carcinogenic chemicals are used in NIH laboratories. The Guidelines should be consulted to identify the proper use conditions required and specific controls to be implemented during normal and complex operations or manipulations involving N-AcO-AAF.

1. Chemical inactivation: No validated method reported.
2. Decontamination: Turn off equipment that could be affected by N-AcO-AAF or the materials used for cleanup. If more than 1 g has been spilled or if there is any uncertainty regarding the procedures to be followed for decontamination, call the NIH Fire Department (dial 116) for assistance. Wipe off surfaces with acetone, then wash with copious quantities of water. Glassware should be rinsed (in a hood) with acetone, followed by soap and water. Animal cages should be washed with water.
3. Disposal: No waste streams containing N-AcO-AAF shall be disposed of in sinks or general refuse. Surplus N-AcO-AAF or chemical waste streams contaminated with N-AcO-AAF shall be handled as hazardous chemical waste and disposed of in accordance with the NIH chemical waste disposal system. Nonchemical waste (e.g., animal carcasses and bedding) containing N-AcO-AAF shall be handled and packaged for incineration in accordance with the NIH medical-pathological waste disposal system. Potentially infectious waste (e.g., tissue cultures) containing N-AcO-AAF shall be disinfected by heat using a standard autoclave treatment and packaged for incineration, as above. Burnable waste (e.g., absorbent bench top liners) minimally contaminated with N-AcO-AAF shall be handled as potentially infectious waste and packaged for incineration, as above. Absorbent materials (e.g., associated with spill cleanup) grossly contaminated shall be handled in accordance with the chemical waste disposal system. Radioactive waste containing N-AcO-AAF shall be handled in accordance with the NIH radioactive waste disposal system.
4. Storage: Store stock quantities of solid material at -20°C.

Monitoring and Measurement Procedures Including Direct Field Measurements and Sampling for Subsequent Laboratory Analysis

Since N-AcO-AAF is strictly a laboratory chemical, methods for field sampling and measurement have not been developed.

1. Sampling: N-AcO-AAF is unstable and is not likely to be detected as the parent compound on solvent extraction (Gutmann et al., 1975).
2. Separation and analysis: There is no reliable procedure since chromatography is accompanied by considerable decomposition (Gutmann and Erickson, 1969, 1972). A colorimetric method developed for 2-acetylaminofluorene (Westfall and Morris, 1947) can probably be adapted for determination of N-AcO-AAF after hydrolysis, but there are no data to this effect.

Biological Effects (Animal and Human)

1. Absorption: No data. Since N-AcO-AAF produces tumors preferentially at the site of application, it is probably less well absorbed than 2-acetylaminofluorene but rather reacts topically with tissue constituents.
2. Distribution: No data.
3. Metabolism and excretion: No data.
4. Toxic effects: There are no data on acute LD50. No toxic effects have been reported.
5. Carcinogenic effects: N-AcO-AAF, when applied topically or parenterally, induces tumors at the site of application in rodents (skin, subcutaneous injection site) probably by direct reaction with tissue constituents. Oral administration of N-AcO-AAF has not been practiced in carcinogenicity studies because of its reactivity.
6. Mutagenic and teratogenic effects: N-AcO-AAF is a strong mutagen in in vitro systems. There are no data concerning its teratogenicity.

Emergency Treatment

1. Skin and eye exposure: For skin exposure, remove contaminated clothing and wash skin with soap and water. For eye exposure, irrigate immediately with copious quantities of running water for at least 15 minutes.
2. Ingestion: Drink plenty of water. Induce vomiting.
3. Inhalation: Remove victim promptly to clean air. Administer rescue breathing if necessary.

4. Refer to physician.

References

- Gutmann, H.R., and R.R. Erickson. 1969. The conversion of the carcinogen N-hydroxy-2-fluorenylacetamide to o-amidophenols by rat liver in vitro. J Biol Chem 244:1729-1740.
- Gutmann, H.R., and R.R. Erickson. 1972. The conversion of the carcinogen N-hydroxy-2-fluorenylacetamide to o-amidophenols by rat liver in vitro: Substrate specificity and mechanism of the reaction. J Biol Chem 247:660-666.
- Gutmann, H.R., D. Malejka-Giganti, and R. McIver. 1975. Identification of carcinogenic acetates of fluorenylhydroxamic acids by high pressure liquid chromatography. J Chromatogr 115:71-78.
- Westfall, B.B., and H.P. Morris. 1947. Photometric estimation of N-acetyl-2-aminofluorene. J Natl Cancer Inst 8:17-21.