

Material Safety Data Sheet

N-Chlorosuccinimide 99%

【Name】

N-Chlorosuccinimide

【Iupac name】

1-chloropyrrolidine-2,5-dione

【CAS Registry number】

[128-09-6](#)

【Synonyms】

2,5-Pyrrolidinedione, 1-chloro-
Chlorosuccinimide
NCS
Pyrrolidinedione, 1-chloro-
Succinchlorimide

【EINECS(EC#)】

[204-878-8](#)

【Molecular Formula】

[C4H4ClNO2 \(Products with the same molecular formula\)](#)

【Molecular Weight】

133.53

【Inchi】

InChI=1/C4H4ClNO2/c5-6-3(7)1-2-4(6)8/h1-2H2

【InChIKey】

JRNVZBWKYDBUCA-UHFFFAOYSA-N

【Canonical SMILES】

C1CC(=O)N(C1=O)Cl

【MOL File】

128-09-6.mol

Chemical and Physical Properties

【Appearance】

white to off-white crystalline powder

【Density】

1.5 g/cm³

【Melting Point】

144-150°C

【Boiling Point】

200.5 °C at 760 mmHg

【Refractive Index】

1.532

【Flash Point】

75.1 °C

【Water】

Slightly soluble

【Solubilities】

Slightly soluble

【Color/Form】

Orthorhombic crystals

PLATES FROM CARBON TETRACHLORIDE

White crystalline powder

【Stability】

Stable at room temperature in closed containers under normal storage and handling conditions.

【HS Code】

29251995

【Storage temp】

Store in a cool, dry place. Do not store in direct sunlight. Store in a tightly closed container.

Store protected from moisture.

【Spectral properties】

IR: 4273 (Coblentz Society Spectral Collection)

NMR: 6226 (Sadler Research Laboratories Spectral Collection)

MASS: 4080 (National Bureau of Standards EPA-NIH Mass Spectra Data Base, NSRDS-NBS-63)

【Computed Properties】

Molecular Weight:133.53306 [g/mol]

Molecular Formula:C₄H₄ClNO₂

XLogP3-AA:-0.2

H-Bond Donor:0

H-Bond Acceptor:2

Rotatable Bond Count:0

Tautomer Count:3

Exact Mass:132.993056

Monoisotopic Mass:132.993056

Topological Polar Surface Area:37.4

Heavy Atom Count:8

Formal Charge:0

Complexity:129

Isotope Atom Count:0

Defined Atom Stereocenter Count:0

Undefined Atom Stereocenter Count:0

Defined Bond Stereocenter Count:0

Undefined Bond Stereocenter Count:0
Covalently-Bonded Unit Count:1
Feature 3D Acceptor Count:2
Feature 3D Ring Count:1
Effective Rotor Count:0.6
Conformer Sampling RMSD:0.4
CID Conformer Count:1

Safety and Handling

【Hazard Codes】

C:Corrosive

【Risk Statements】

R22;R34

【Safety Statements】

S26;S37/39

【HazardClass】

8

【Hazard Note】

Irritant

【Safety】

Hazard Codes: ?  C,  Xi

Risk Statements: 22-34?

R22:Harmful if swallowed.?

R34:Causes burns.

Safety Statements: 26-36/37/39-45-37/39?

S26: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.?

S36/37/39:Wear suitable protective clothing, gloves and eye/face protection.?

S45:In case of accident or if you feel unwell, seek medical advice immediately (show the label whenever possible.)?

S37/39:Wear suitable gloves and eye/face protection.

【PackingGroup】

III

【Sensitive】

Moisture Sensitive

【Skin, Eye, and Respiratory Irritations】

STRONG SKIN IRRITANT.

【Transport】

25kgs

【Fire Potential】

NANJING SURU CHEMICAL CO.,LTD
www.suruchem.com
TEL:86-025-52406782 FAX:86-025-52412030

Stored as a dust it heats spontaneously.

【Reactivities and Incompatibilities】

Explosive reaction with aliphatic alcohols, benzylamine, or hydrazine hydrate.

【Protective Equipment and Clothing】

STRONG SKIN IRRITANT.

【Specification】

?N-Chlorosuccinimide (CAS NO.128-09-6) is a white crystal, soluble in water and alcohols, it can be used as pharmaceutical intermediates, organic synthesis chlorinating agent, it can also be used to prepare rubber additives, synthesis as chlorinating agent, antibiotic drugs intermediates.

?Production method is through the ammoniated acid chloride derived. Through dropping ammonia, react with succinic acid, stirring heated at 102°C steam to get rid of water. Vacuum distillation, collecting 180°C after the distillate to get succinimide. Molten succinimide increased to acetic acid aqueous solution, stirring cooled to 0-5°C, dropping sodium hypochlorite, control reaction in the 8°C below (otherwise there is risk of explosion). To clarify the reaction solution that is reached when the end point, centrifugation, filter cake and washing to neutral, drying, drying to get.

【Report】

EPA Genetic Toxicology Program.

【Disposal Methods】

SRP: At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices.