



# **Sodium Chloroacetate** (2016)

I. IDENTIFICATION (1-3)

Chemical Name: Sodium chloroacetate

Synonyms: Monoxone, sodium monochloroacetate, chloroacetic

acid, sodium salt CAS Number: 3926-62-3

Molecular Formula: C<sub>2</sub>H<sub>2</sub>ClO<sub>2</sub>Na

Structural Formula:

# II. CHEMICAL AND PHYSICAL PROPERTIES (1,3-8)

Physical State: White to off-white crystalline powder with

pungent smell

Molecular Weight: 116.48

Conversion factors: 1 ppm =  $4.76 \text{ mg/m}^3$ ; 1 mg/m<sup>3</sup> = 0.21 ppmMalting Point: 170 °C (338 °F). Decomposes glowly at 150 °C

Melting Point: 170 °C (338 °F). Decomposes slowly at 150 °C

by localized heating Boiling Pt: Not available

Vapor Pressure: 0.865 mm Hg @ 25 °C, 1 mm Hg @ 43 °C

Saturated Vapor Concentration: 1138 ppm @ 25 °C

(77°F) (calculated)

Specific gravity: Not available

Vapor Density (air =1): 4.0

Odor: Pungent

Odor threshold: Not available

Flammability Limits: LFL and UFL - Not available

Flash Point (closed cup):  $270 \, ^{\circ}\text{C} (518 \, ^{\circ}\text{F})$ 

Solubility: 820 g/L @ 20 °C insoluble in Alcohol, Ether,

Acetone, and Chloroform

pH = 4.5-4.9 @ 50g/L and 20 °C

Stability and Reactivity: Stable at normal temperatures and pressures. Incompatible with oxidizing agents, reducing

agents.

III. USES<sup>(2,3)</sup>

Sodium chloroacetate is used as a contact herbicide and a component in other herbicides, an intermediate in the production of carboxymethyl-cellulose, and other synthetic organic chemicals.

#### IV. ANIMAL TOXICITY DATA

A. Acute Toxicity

# 1. Lethality Data

Species	Route	LD <sub>50</sub> mg/kg
Rat	Oral	76-580 <sup>(2,3,9)</sup>
Rat	Dermal	>2000 mg/kg <sup>(2,3)</sup>
Mouse	Oral	165-339 <sup>(2,3,9)</sup>
Golden Hamster	Oral	245 <sup>(2,3)</sup>
Guinea Pig	Oral	80-115 <sup>(2,3,9)</sup>
Rabbit	Oral	156 <sup>(2,3,9)</sup>

In one study systemic effects to Sprague-Dawley rats (M/F, numbers per group not indicated) given single doses of sodium chloroacetate at 94, 282, or 470 mg/kg bw demonstrated increased sodium concentration in urine, increased potassium concentration in plasma, and reduced glutathione level in the liver at the highest dose; 2/3 of males died within 24 hours of treatment in the middle and high dose groups.

## 2. Eye Irritation

A 25% aqueous solution of sodium chloroacetate was mildly irritating to eyes in rabbits. (2)

## 3. Skin Absorption

Sodium chloroacetate has not been shown to be absorbed in toxicologically significant quantities through the skin. (2,3,10)

## 4. Skin Irritation

Sodium chloroacetate was shown to be a non- to moderate skin irritant but not corrosive to the skin. (3,4,15)

## 5. Skin Sensitization

Not indicated to be a sensitizer. (2,3)

#### 6. Acute Inhalation Toxicity

No cases of "acute intoxication from MCA (sodium salt)" have been located in the literature. (10)

#### B. Subacute Toxicity

No information available

#### C. Subchronic Toxicity

Sprague-Dawley rats were given repeated oral doses (by gavage) for 90 days at 0, 15, 30, 60, or 120 mg/kg/day (10 animals/dose). In the highest dose group, 80 % of males and 30% of females died. In both sexes of the 60 mg/kg/day group there were significant increases in liver and kidney weights. In all dose groups there were changes to hematological parameters, and numerous clinical chemistry parameters (increases in urea nitrogen, creatinine, calcium and phosphate, increases in ALT and AST in serum). In males of the 60 mg/kg/day dose group there was a significant increase in chronic nephropathy and spleen pigmentation as well as a dose-dependent increase in vacuolated hepatocytes. The LOAEL is concluded to be 15 mg/kg/day. (2,3,11)

### D. Chronic Toxicity/Carcinogenicity

There was no evidence of carcinogenic activity in F344N rats or B6C3F mice at 15 or 30 mg/kg, or 50 or 100 mg/kg respectively in an NTP study using the parent compound monochloroacetic acid (MCA (CAS 79-11-8). Neither structurally similar MCA or sodium chloroacetate are considered likely potential human carcinogens. (10,12,13)

#### E. Reproductive/Developmental Toxicity

Rats (strain not indicated) were dosed by gavage with 17-140 mg/kg bw (0, 17, 35, 70, or 140 mg/kg sodium chloroacetate) on gestation days 6-15. The maternal NOEL was 17 mg/kg/day and the maternal NOAEL was 70 mg/kg/day (mean adjusted percentage bodyweight gain). Cardiovascular malformations, and other soft tissue malformations were seen at the high-dose group with no effects seen at other dose levels.<sup>(2)</sup>

#### F. Genotoxicity/Mutagenicity

Ames (TA 1535, 1537, 1538, 98, 100) bacterial test: was negative (+/- S9); HPRT/V79 CHL test was negative (+/-S9); Mice (Swiss strain) micronucleus test was negative. (2,5,10,14)

#### G. Metabolism/Pharmacokinetics

After absorption, monochloroacetic acid (parent compound CAS 79-11-8) is converted to thiodiacetic acid and glycolic acid and is accumulated in the liver and kidneys of rats. (10,15) Metabolism of sodium monochloroacetate is expected to have a similar pharmacokinetic profile.

### V. HUMAN USE AND EXPERIENCE

There are a number of case studies of the parent compound, monochloroacetic acid (MCA), involving corrosion of skin and eyes and fatalities related to skin absorption of toxicologically significant amounts of MCA and a health-based target concentration of 0.1 mg/L was calculated for MCA in drinking water<sup>(10)</sup> although Health Canada and Environment Canada have categorized MCA as not entering the environment at levels that may be hazardous to human health.<sup>(16)</sup> There are, however, no similar data or epidemiological reports for sodium chloroacetate.<sup>(2-4)</sup>

#### VI. RATIONALE

Sodium chloroacetate metabolizes quickly to monochloroacetic acid (MCA) when given orally. It has a moderate acute oral toxicity in rats but was not shown to be an eye or skin irritant or dermal sensitizer and was negative in genotoxicity testing. There is a lack of inhalation or chronic exposure data. A 90-day rat oral subchronic study using MCA is considered to be the pivotal study in recommending a WEEL. The study indicated a LOAEL of 15 mg/kg/day with the primary systemic toxicological endpoints related to liver and kidney toxicity. Based on this, a WEEL of 0.5 ppm, 8-hr TWA is recommended as being sufficiently protective.

#### VII. RECOMMENDED WEEL

8-hr time-weighted average (TWA): 0.5 ppm (2.5 mg/m<sup>3</sup>)

This WEEL value was originally established in 2005. No significant new literature was identified since 2005 that supports a change to the recommended WEEL value.

## **VIII. REFERENCES**

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