

## SODIUM CITRATE

This dossier on sodium citrate presents the most critical studies pertinent to the risk assessment of sodium citrate in its use in water treatment systems. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the OECD-SIDS documents on citric acid (OECD 2001a,b) and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sodium citrate is classified as a **tier 1** chemical and requires a hazard assessment only.

### 1 BACKGROUND

Sodium citrate is readily biodegradable. It is not expected to bioaccumulate. Due to its high water solubility, citric acid is unlikely to adsorb to soil or sediment. Sodium citrate is of low toxicity concern to aquatic organisms.

### 2 CHEMICAL NAME AND IDENTIFICATION

**Chemical Name (IUPAC):** Trisodium 2-hydroxypropane-1,2,3-tricarboxylate dihydrate

**CAS RN:** 6132-04-3

**Molecular formula:**  $C_6H_5Na_3O_7 \cdot 2H_2O$  or  $C_6H_9Na_3O_9$

**Molecular weight:** 294.10 g/mol

**Synonyms:** Sodium citrate; sodium citrate dihydrate; sodium citrate, anhydrous; anhydrous sodium citrate; trisodium citrate dihydrate; trisodium 2-hydroxypropane-1,2,3-tricarboxylate dihydrate

### 3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

**Table 1 Overview of the Physico-chemical Properties of Sodium Citrate**

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Crystalline solid	2	ECHA
Melting Point	>150°C (pressure not reported)	2	ECHA
Boiling Point	Not available; decomposition	-	ECHA
Density	1857 kg/m <sup>3</sup> @ 20°C	2	ECHA
Vapour Pressure	0 Pa @ 25°C	2	ECHA
Partition Coefficient (log K <sub>ow</sub> )	-1.72 (temperature not provided)	4	ECHA

Property	Value	Klimisch score	Reference
Water Solubility	@ 400 – 700 g/L @ 20-25 °C	4	ECHA
Dissociation constant (pKa)	3.13, 4.76, 6.4 @ 25 °C	2	ECHA

#### 4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium citrate.

NICNAS has assessed sodium citrate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment<sup>1</sup>.

**Table 2 Existing International Controls**

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

#### 5 ENVIRONMENTAL FATE SUMMARY

##### A. Summary

Sodium citrate is readily biodegradable. It is not expected to bioaccumulate. Due to its high water solubility, citric acid is unlikely to adsorb to soil or sediment.

##### B. Partitioning

Sodium citrate lacks any of the functional group that are susceptible to hydrolysis in aqueous solution.

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<sup>1</sup> <https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=6132-04-3%2C+>

### C. Biodegradation

Sodium citrate dissociates in aqueous solutions to sodium ( $\text{Na}^+$ ) and citrate ( $\text{C}_6\text{H}_5\text{O}_7^-$ ) ions. Sodium citrate can be considered readily biodegradable based on the results of the ready and inherent aerobic biodegradation studies on citric acid listed in Table 3.

If a chemical is found to be inherently or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

**Table 3 Biodegradation Studies on Citric Acid (OECD 2001a,b)**

Test System	Results*	Notes	Klimisch Score
Modified Sturm	97% ( $\text{CO}_2$ evolution); 100% (DOC removal)	Readily biodegradable; exposure period not stated	2
Closed Bottle Test	$\text{BOD}_{30}/\text{COD}$ Ratio = 90%	Readily biodegradable	2
$\text{BOD}_5/\text{COD}$ Ratio	$\text{BOD}_5 = 526$ mg; $\text{COD} = 728$ mg; $\text{BOD}_5/\text{COD}$ Ratio = 0.72	Readily biodegradable; concentration of test substance and activated sludge not stated	2
$\text{BOD}_1/\text{ThOD}$ Ratio	$\text{BOD}_1/\text{ThOD}$ Ratio = 13%	-	2
$\text{BOD}_{20}/\text{ThOD}$ Ratio	$\text{BOD}_{20}/\text{COD}$ Ratio = 98%	Readily biodegradable; initial test substance concentration 720 mg/L	2
Zahn-Wallen Test	85%, 1 day (DOC removal)	Inherently biodegradable	2
Zahn-Wallen Test	98%, 7 days (DOC removal)	Inherently biodegradable	
Coupled Units Test	93% (COD removal)	Ultimately biodegradable; exposure period not stated	2

### D. Environmental Distribution

No experimental data are available for sodium citrate or citric acid. Using KOCWIN program in EPISuite™ (USEPA, 2016), the estimated  $K_{oc}$  value for citric acid from the  $K_{ow}$  value of -1.08 is 0.3617 L/kg.

If released to soil, based on this negligible  $K_{oc}$  value, this substance is unlikely to adsorb to soil and would be highly mobile. If released to water, based on a negative  $K_{ow}$  value and high water solubility, this substance is unlikely to adsorb to suspended solids and would preferentially partition to the water column.

### E. Bioaccumulation

The log  $K_{ow}$  for sodium citrate is -1.72. Thus, sodium citrate is not expected to bioaccumulate.

As noted above, sodium citrate dissociates in aqueous solution to the metal ion ( $\text{Na}^+$ ) and citrate ions ( $\text{H}_7\text{C}_6\text{O}_7^-$ ). Citrate is found in all eukaryotic cells as an intermediate of the TCA cycle, which is

part of the basic metabolic pathway that generates useable energy from carbohydrates, proteins and fats. Citric acid is formed and broken down in the course of this cycle at very high rates (ECHA).

An estimated BCF for citric acid was 3.2 L/kg (ECHA) [Kl. Score = 2]. The weight of evidence of the low estimated BCF, biodegradability and role in cell metabolism indicate that citric acid is extremely unlikely to bioaccumulate (ECHA).

## 6 ENVIRONMENTAL EFFECTS SUMMARY

### A. Summary

Sodium citrate is of low toxicity concern to aquatic organisms.

### B. Aquatic Toxicity

#### Acute Studies

No studies are available on sodium citrate.

The 48-hour LC<sub>50</sub> values for citric acid in *Leuciscus idus melanotus* (golden orfe) from two separate laboratories were 440 mg/L and 760 mg/L (ECHA) [Kl. scores = 2]. The 96-hour LC<sub>50</sub> for citric acid in *Lepomis macrochirus* (fathead minnow) is >100 mg/L (ECHA) [Kl. score = 2].

The 24-hour EC<sub>50</sub> value for citric acid in *Daphnia* is 85 mg/L in un-neutralised test solution and 1,535 mg/L in a neutralised solution (OECD, 2001a,b; ECHA). [Kl. score = 2]

The 8-day toxicity threshold value (EC<sub>0</sub>) for citric acid in *Scenedesmus quadricauda* is 640 mg/L (ECHA; OECD, 2001a,b). [Kl. score = 2]

#### Chronic Studies

No studies are available. As outlined in ECHA, testing is not considered necessary because:

- Short-term toxicity to aquatic organisms is low.
- Risk characterisation ratios based on PNEC<sub>aquatic</sub> calculated using the short-term data are <1.
- The parent acid substance is naturally occurring in aquatic organisms and so is the counter ion.

### C. Terrestrial Toxicity

No studies are available. The substance has a negative log K<sub>ow</sub> value and therefore, partitioning to the terrestrial compartment is expected to be minimal (ECHA).

## **7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN**

### **A. PBT Categorisation**

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium citrate is readily biodegradable; thus, it does not meet the screening criteria for persistence.

The log  $K_{ow}$  values for sodium citrate are -1.72. Thus, sodium citrate does not meet the screening criteria for bioaccumulation.

There are no chronic aquatic toxicity studies on citric acid or sodium citrate. The acute  $EC_{50}$  values for citric acid are >1 mg/L in fish and invertebrates. Thus, it does not meet the screening criteria for toxicity.

The overall conclusion is that sodium citrate is not a PBT substance.

### **B. Other Characteristics of Concern**

No other characteristics of concern were identified for sodium citrate.

## 8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment <sup>1</sup>	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required <sup>3</sup>
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity <sup>2</sup>	Chronic Toxicity <sup>2</sup>	
Sodium Citrate	6132-04-3	Not a PBT	No	No	No	No	No	No	1	1	1

**Footnotes:**

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

**Notes:**

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

## 9 REFERENCES, ABBREVIATIONS AND ACRONYMS

### A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: <https://echa.europa.eu/information-on-chemicals/registered-substances>

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

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OECD. (2001b). Screening Information Dataset (SIDS) Initial Assessment Report for Citric acid (CAS No. 77-92-9), UNEP Publications).

USEPA. (2016). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: <https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface>.

### B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BOD	biological oxygen demand
COC	constituent of concern
COD	chemical oxygen demand
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union

g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m <sup>3</sup>	kilograms per cubic metre
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
mg	milligrams
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
TCA	tricarboxylic acid
ThOD	theoretical oxygen demand
USEPA	United States Environmental Protection Agency