SODIUM GLUCONATE

This dossier on sodium gluconate presents the most critical studies pertinent to the risk assessment of this substance in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from Organization for Economic Cooperation and Development Screening Information Dataset (OECD SIDS) (OECD, 2004). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

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

1 BACKGROUND

Sodium gluconate is the organic sodium salt of gluconic acid. Sodium gluconate is a chelator that forms stable complexes with various ions and ultimately prevents these ions from engaging in chemical reactions. Gluconates are naturally occurring substances that freely dissociate to the gluconate anion and its respective cations. Gluconates is used as a chelating agent in many cleaning products, industrial applications, and foodstuffs.

Sodium gluconate is readily biodegradable. It is not expected to bioaccumulate, and it has low potential to adsorb to sediment and soil. In addition to this, sodium gluconate has a low acute toxicity to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sodium D-gluconate

CAS RN: 527-07-1

Molecular formula: $C_6H_{11}NaO_7$

Molecular weight: 218.14g/mol

Synonyms: SODIUM GLUCONATE, Sodium D-gluconate 527-07-1, D-Gluconic acid, monosodium salt,D-Gluconic acid sodium salt

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 Gluconate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Dry, white, crystalline powder	-	PubChem

Property	Value	Klimisch score	Reference
Melting Point	205-209 °C (pressure not provided)	-	OECD, 2004
Boiling Point	613.1 °C (pressure not provided)	-	OECD, 2004
Density	1790 kg/m^3	-	PubChem
Vapor Pressure	Negligible @ 25 °C	-	OECD, 2004
Partition Coefficient (log K_{ow})	-5.99	-	OECD, 2004
Water Solubility	590 g/L @ 25 °C	-	OECD, 2004
Dissociation constant (pKa)	3.70	-	OECD, 2004

Sodium gluconate is the sodium salt of gluconic acid. Gluconic acid is a naturally occurring weak acid and its dissociation in water is expected to be complete.

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 gluconate.

NICNAS has assessed sodium gluconate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[1].

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

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=527-07-1

5 ENVIRONMENTAL FATE PROPERTIES

A. Summary

Sodium gluconate is readily biodegradable. It is not expected to bioaccumulate, and it has low potential to adsorb to sediment and soil.

B. Partitioning

Sodium gluconate is highly soluble in water. Volatilization from water or moist soil surfaces is not expected to be an important fate process based upon its water solubility and that it is a salt. It is not expected to volatilize from dry soil surfaces based upon its estimated negligible vapour pressure.

C. Biodegradation

Sodium gluconate is readily biodegradable under both aerobic and anaerobic conditions. In an aerobic closed bottle test of sodium gluconate, the biodegradation was 89% expressed as the Theoretical Oxygen Demand after 28 days; while under anaerobic conditions, 100% of sodium gluconate was determined as degraded after 35 days. These data demonstrate that gluconates are readily biodegradable both under aerobic and anaerobic test conditions (OECD, 2004).

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

D. Environmental Distribution

No experimental data are available for adipic acid. Using KOCWIN in EPISuite™ (USEPA, 2018), the estimated K_{oc} value from log K_{ow} is 0.0001046 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 10 L/kg. Based on these values, sodium gluconate has a low potential for adsorption to soil and sediment and is expected to have very high mobility in soil.

E. Bioaccumulation

Based on a log K_{ow} value of -5.99, sodium gluconate has a very low potential for bioaccumulation. This is further supported by metabolic in vivo studies showing that gluconate is readily catabolized or utilized for glucose synthesis (OECD, 2004).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium gluconate has low acute toxicity to aquatic organisms. No chronic toxicity studies have been reported.

B. Aquatic Toxicity

<u>Acute Studies</u>

Table 3 presents the results of acute aquatic toxicity studies conducted on Sodium gluconate.

Table 3 Acute Aquatic Toxicity Studies on Sodium Gluconate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
*Oryzias latipes (*Fish, freshwater)	96-hr LC_{50}	>100	-	OECD, 2004
Daphnids magna (Crustacea)	24-48h NOEC	>1000	-	OECD, 2004
Selenastrum capricornutum (Algae)	24-72 h $NOEC_r$ 24-72 h E_rC_{50}	560 >1000	-	OECD, 2004

Chronic Studies

No studies reported.

C. Terrestrial Toxicity

No terrestrial toxicity data for gluconates are available. However, the demonstrated biodegradability and the low intrinsic toxicity of gluconates that was observed for aquatic organisms, data on animal toxicokinetic and metabolism (cfr. human toxicology) and their role in mammalian carbohydrate metabolism may predict also a low effect on terrestrial organisms. Therefore, no terrestrial toxicity studies would be required (OECD, 2004).

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

The estimated log K_{ow} for sodium gluconate is -5.99. Thus, sodium gluconate does not meet the criteria for bioaccumulation.

There are no chronic aquatic toxicity studies on sodium gluconate. The acute $E(L)C_{50}$ values are >1 mg/L. Thus, sodium gluconate does not meet the screening criteria for toxicity.

Therefore, sodium gluconate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium gluconate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			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 [2]	Chronic Toxicity[2]	
Sodium Gluconate	527-07-1	Not a PBT	No	No	No	No	No	No	1	No data	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.

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USEPA. (2018). 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
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
IMAP	Inventory Multitiered Assessment and Prioritisation
IUPAC	International Union of Pure and Applied Chemistry

KOCWIN	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
NOEC	no observed effect concentration
Pa	Pascal
PBT	Persistent Bioaccumulative Toxic
QSAR	quantitative structure-activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency