# EDETIC ACID

This dossier on edetic acid (also known as ethylene diaminetetraacetic acid [EDTA]) presents the most critical studies pertinent to the risk assessment of EDTA in its use in coal seam gas extraction activities. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from 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 – EDTA is classified as a **tier 1** chemical and requires a hazard assessment only.

## 1 BACKGROUND

EDTA is an aminopolycarboxylic acid. This white, water-soluble solid is widely used to bind to iron and calcium ions. It binds these ions as a hexadentate ("six-toothed") chelating agent. EDTA is produced as several salts, notably disodium EDTA, sodium calcium edetate, and tetrasodium EDTA ($Na_4EDTA$).

EDTA is not readily or inherently biodegradable, but it can under certain conditions (*i.e.*, alkaline pH), which is realistic under environmental surface water conditions, be degraded. Therefore, it can be concluded that EDTA is ultimately biodegradable under such environmental conditions. It is highly soluble in water and is not expected to adsorb to soil or sediment. EDTA has a low potential for bioaccumulation.

EDTA is of low toxicity concern to aquatic and terrestrial organisms. However, the mode-of-action of EDTA in aquatic systems involves disturbances of metal metabolism; hence the complex formation properties of EDTA need to be taken into account.

## 2 CHEMICAL NAME AND IDENTIFICATION

**Chemical Name (IUPAC)**: 2,2',2'',2'''-(ethane-1,2-diyldinitrilo)tetraacetic acid

**CAS RN**: 60-00-4

**Molecular formula:** $C_{10}H_{16}N_2O_8$

**Molecular weight:** 292.24 g/mol

**Synonyms**: Edetic acid; ethylenediaminetetraacetic acid; EDTA; Glycine, N,N'-1,2-ethanediylbis[N-(carboxymethyl)-

## 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 EDTA**

| Property | Value | Klimisch score | Reference |
|---|---|---|---|
| Physical state at 20°C and 101.3 kPa | Odourless white solid | 2 | ECHA |
| Melting Point | Decomposes @ > 220 °C | 2 | ECHA |
| Boiling Point | Decomposes before boiling | - | ECHA |
| Density | 1460 kg/$m^3$ @ 20 °C | 2 | ECHA |
| Vapour Pressure | 1.99 x $10^{-10}$ Pa @ 25 °C | 2 | ECHA |
| Partition Coefficient (log $K_{ow}$) | -3.86 @ 25 ° C | 2 | ECHA |
| Water Solubility | 0.4 g/L @ 20°C | 2 | ECHA |
| Dissociation constant pKa | -0.12-10.44 @ 20°C with different electrolytes, ion strength and electrodes | 2 | ECHA |

The substances in the EDTA and its salts group, when in solution, are expected to dissociate into the same anionic species of EDTA in the environment (EU, 2004).

## 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 EDTA.

**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

EDTA is not readily or inherently biodegradable, but it can under certain conditions (*i.e.*, alkaline pH), which is realistic under environmental surface water conditions, be degraded. Therefore, it can be concluded that EDTA is ultimately biodegradable under such environmental conditions. It is highly soluble in water and is not expected to adsorb to soil or sediment. EDTA has a low potential for bioaccumulation.

### B. Partitioning

After evaporation or exposure to the air, EDTA will be rapidly degraded by photochemical processes. However, photodegradation is not considered to be an important environmental fate process since the substance is not expected to evaporate into the atmosphere due to the low vapor pressure. Abiotic hydrolysis is not relevant, since neither strong acids nor alkalis cause any degradation (ECHA).

### C. Biodegradation

EDTA is not readily biodegradable according to OECD criteria. In standard OECD 301D ready biodegradability tests with natural river and lake water less than 60% biodegradation was observed for EDTA species after 28 day incubation time. In these same tests however > 60% biodegradation was observed when prolonged to 60 days indicating that EDTA and other EDTA species are inherently and ultimately biodegradable in a ready biodegradation test under enhanced conditions (ECHA). [Kl. Score = 1 or 2, depending on study].

Several intrinsic/extrinsic factors are known to influence the biodegradation behaviour including pH, adaptation, influences of the stability constant and degradation pathway. For example, it could be shown that a change of the pH-value has significant influence on the biodegradability of EDTA. In a semi-continuous activated sludge (SCAS) test (OECD 302 A) biodegradation of EDTA could be observed at pH 8-9, but not significantly at pH 6.5 (ECHA) [Kl. Score = 2]. Similar results obtained in a dissolved organic carbon (DOC) removal test according to the principles of the OECD guideline 301 using natural surface water from the river Rhine as inoculum. After 60 days up to 100 % EDTA was degraded at pH 8.5 but less than 10 % at pH 6.5 (ECHA). [Kl. Score = 2]. These slightly alkaline conditions are realistic in environmental surface water compartments (ECHA).

As a chelating agent, EDTA forms complexes with cationic ions. Fundamental EDTA exists naturally as a mixture of chelate complexes (ECHA). EDTA complexes are usually stable water-soluble complexes with high formation (or stability) constants. There are data suggesting that under alkaline conditions EDTA complexed with calcium ions can be biodegraded which could be relevant for certain surface waters. However, in surface waters EDTA is preferably complexed with heavy metal ions and no biological degradation is expected for these complexes (OECD, 2004). Therefore, EDTA is regarded as not biodegradable in surface waters. However, available data indicate that EDTA species, especially iron complexes, are to certain degree photolysable in water and soil (EU, 2004).

Two studies are available investigating the biodegradability of EDTA in soil. For the determination of biodegradation in soil non-standard investigations under various conditions show that EDTA can be biodegraded in soil under aerobic conditions. The rate of EDTA degradation was determined in different agricultural soils after 4 - 45 weeks of exposure. While degradation rate was 10-12% only after 4 weeks the degradation continued showing 32-45% degradation after 15 weeks and >= 65% after 45 weeks incubation time. This indicates that EDTA is (slowly) biodegradable in soil and thus not persistent in the terrestrial compartment (ECHA). [Kl. Score = 2].

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

### D. Environmental Distribution

No experimental data are available for EDTA. Using KOCWIN in EPISuite™ (USEPA, 2019), the estimated $K_{oc}$ value from the molecular connectivity index (MCI) is 312.7 L/kg. Based on this value and high water solubility, EDTA has a low potential for adsorption to soil and is expected to have a moderate mobility in soil (ECHA). [Kl. Score = 2]. In addition, the pKa of EDTA is 0.26, indicating that this compound will almost entirely exist in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(PubChem).

### E. Bioaccumulation

Since no study investigating the bioaccumulation potential is available for EDTA, the assessment was based on a study conducted with $Na_4EDTA$ (CAS No. 64-02-8) in a read across approach. At exposures of 0.76 and 0.08 mg/L, $Na_4EDTA$ exhibited extremely low 28-day whole fish bioconcentration factors (BCF) of 1.1 - 1.8 in *Lepomis macrochirus*. These measured values indicate a low potential for bioaccumulation (ECHA). [Kl. Score = 2].

## 6 ENVIRONMENTAL EFFECTS SUMMARY

### A. Summary

EDTA is of low toxicity concern to aquatic and terrestrial organisms. However, the mode-of-action of EDTA in aquatic systems involves disturbances of metal metabolism; hence the complex formation properties of EDTA need to be taken into account.

### B. Aquatic Toxicity

<u>Acute Studies</u>

Table 3 lists the results of acute aquatic toxicity studies conducted on EDTA and its salts (where data for EDTA was unavailable).

**Table 3 Acute Aquatic Toxicity Studies on EDTA**

| Test Species | Endpoint | Results (mg/L) | Klimisch score | Reference |
|---|---|---|---|---|
| *Lepomis macrochirus* (Blue Gill) | 96-hr $LC_{50}$ (mortality) | 401.7 | 2 | ECHA |
| *Daphnia magna* (Daphnid) | 48-hr $EC_{50}$ (mortality) | >114 * | 1 | ECHA |
| *Pseudokirchneriella subcapitata* (Algae) | 72-hr $EC_{50}$ (growth rate) | >100 ** | 1 | ECHA |

*Based on read-across substance ethylenediaminetetraacetic acid iron(III) potassium salt (CAS No. 54959-35-2)
**Based on read-across substance sodium feredetate (CAS No. 15708-41-5)

In short-term tests on fish, EDTA and its salts are more toxic in an uncomplexed form. This can only occur if they are available in over-stoichiometric amounts to the chelants. Under these conditions the complexing agents can cause nutrient deficiency by reducing the essential concentration of different ions. The higher the water hardness the higher is the concentration of EDTA necessary to cause a toxic effect expressed as mortality (OECD, 2004).

As a result, there is a large influence of the speciation to the ecotoxicity of EDTA. Therefore, tests with EDTA metal complexes have to be considered as well. Table 4 provides a summary of the influence of different complexed metal ions on the toxicity of EDTA as investigated with Lepomis macrochirus. In all tests medium hard water with a water hardness of 103 mg/L $CaCO_3$ is used. Effect values are given as $H_4$EDTA (EU, 2004).

**Table 4 Influence of Complex Metal Ions on EDTA Fish Toxicity**

| EDTA Species | 96-hr $LC_{50}$ |
|---|---|
| $Na_4$-EDTA | 374 mg/L |
| Cu-EDTA | 458 mg/L |
| Zn-EDTA | 563 mg/l |
| Mn-EDTA | 11, 940 mg/L |
| $CaNa_2$-EDTA | 1,827 mg/L |
| Mg-EDTA | 2,344 mg/L |

Chronic Studies

Table 5 lists the results of chronic aquatic toxicity studies conducted on EDTA and its salts (where data for EDTA was unavailable).

**Table 5 Chronic Aquatic Toxicity Studies on EDTA**

| Test Species | Endpoint | Results (mg/L) | Klimisch score | Reference |
|---|---|---|---|---|
| *Danio rerio* (Zebra Fish) | 35-d NOEC | >35.1 (>25.7 mg EDTA/L)* | 1 | ECHA |
| *Daphnia magna* (Daphnid) | 21-d NOEC | 25** | 1 | ECHA |
| *Pseudokirchneriella subcapitata* (Algae) | 72-hr $EC_{10}$ (growth rate) | 48.4*** | 1 | ECHA |

*Based on read-across substance sodium calcium edetate (CAS No. 62-33-9)
**Based on read-across substance disodium dihydrogen ethylenediaminetetraacetate (CAS No. 139-33-3)
***Based on read-across substance sodium feredetate (CAS No. 15708-41-5)

### C. Terrestrial Toxicity

Experimental data are available for EDTA or its salts investigating the short-term toxicity to earthworms and terrestrial plants.

In a 14-day OECD Guideline 207 (Earthworm, Acute Toxicity Test) test, the $EC_{50}$ was determined to be 156.46 mg/kg soil dw for EDTA which is based on mortality in earthworms (ECHA). [KI. Score =2].

In a 14-day non-Guideline exposure test, EDTA showed no inhibitory effect on seedling emergence and growth of *Phaseolus vulgaris* up to a concentration of 58.4 mg/kg soil, the established NOEC (ECHA). [Kl. Score = 2].

In a 21-day toxicity test using suitable read across substances, showed an 21d-NOEC values of >= 333 mg/kg soil dw for *Avena sativa*, 160 mg/kg soil dw for *Brassica napus* and 111 mg/kg soil dw for *Glycine max* based on nominal (analytically verified) concentrations, respectively (ECHA). [Kl. Score = 2].

## 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).

EDTA is not readily or inherently biodegradable; thus, it meets the screening criteria for persistence.

The experimental BCF of read-across substance $Na_4EDTA$ in fish is 1.1 – 1.8. Thus, EDTA does not meet the criteria for bioaccumulation.

The lowest NOEC from chronic aquatic toxicity studies is >0.1 mg/L. Acute $EC_{50}$ values in fish, invertebrates, and algae are >1 mg/L. Thus, EDTA does not meet the screening criteria for toxicity.

The overall conclusion is that EDTA is not a PBT substance.

## B. Other Characteristics of Concern

In short-term tests on fish, EDTA and its salts are more toxic in an uncomplexed form. However, in the environment there is no uncomplexed EDTA. Therefore, tests with EDTA metal complexes have to be considered as well. The results show that the toxicity of complexes with the toxic metals Cu and Zn is in the same concentration range as the uncomplexed EDTA. Chelates with non-toxic metals (Mn, Ca, Mg) are much less toxic.

No other characteristics of concern were identified for EDTA .

## 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] | |
| EDTA | 60-00-4 | Not a PBT | No | No | Yes | EDTA is not readily or inherently biodegradable. However, it will biodegrade in alkaline environments (above pH 8) or in soil under aerobic conditions. | 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


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### B. Abbreviations and Acronyms

| | |
|---|---|
| °C | degrees Celsius |
| AICS | Australian Inventory of Chemical Substances |
| BCF | bioconcentration factor |
| COC | constituent of concern |

| | |
|---|---|
| DOC | dissolved organic carbon |
| DEWHA | Department of the Environment, Water, Heritage and the Arts |
| EC | effective concentration |
| ECb | effective concentration (biomass) |
| ECHA | European Chemicals Agency |
| ECr | effective concentration (growth rate) |
| EU | European Union |
| g/L | grams per litre |
| hPa | hectopascal |
| IUPAC | International Union of Pure and Applied Chemistry |
| $kg/m^3$ | kilogram per cubic metre |
| kPa | kilopascal |
| LC | lethal concentration |
| NOEC | no observed effective concentration |
| OECD | Organisation for Economic Co-operation and Development |
| Pa | Pascal |
| PBT | Persistent, Bioaccumulative and Toxic |
| RAR | Risk Assessment Report |
| REACH | Registration, Evaluation, Authorisation and Restriction of Chemicals |
| SGG | Synthetic Greenhouse Gases |
| TG | test guideline |
| TOD | Total oxygen demand |