

ADIPIC ACID

This dossier on adipic acid presents the most critical studies pertinent to the risk assessment of adipic acid in its use in water treatment systems. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA) and from the OECD-SIDS document on adipic acid (OECD, 2004). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

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

1 BACKGROUND

Adipic acid is readily biodegradable. It is not expected to bioaccumulate, and it has low potential to adsorb to sediment and soil. Adipic acid is moderately toxic to aquatic organisms on an acute and chronic basis.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Hexanedioic acid

CAS RN: 124-04-9

Molecular formula: C₆H₁₀O₄

Molecular weight: 146.1 g/mol

Synonyms: Adipic acid; hexanedioic acid

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 Adipic Acid

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, crystalline solid		PubChem
Melting Point	150.85°C @ 101.3 kPa		PubChem
Boiling Point	337.5°C @ 101.3 kPa		PubChem
Density	1360 kg/m ³ @ 25°C		PubChem
Vapour Pressure	9.7 Pa @ 18.5°C		PubChem
Partition Coefficient (log K _{ow})	0.093 [experimental]		PubChem

Property	Value	Klimisch score	Reference
Water Solubility	23 g/L @ 25°C		PubChem
Dissociation constants (pKa)	pK1 = 4.43 @ 25°C pK2 = 5.42		PubChem

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 adipic acid.

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

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

B. Partitioning

Volatilization of adipic acid from moist soil surfaces or water surfaces is not expected to be an important fate process given a Henry's Law constant of 0.0616 Pa*m³/mol. Acetic acid is not expected to volatilize from dry soil surfaces based upon its vapour pressure.

Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions (PubChem).

C. Biodegradation

Adipic acid was readily biodegradable in an OECD 301 D test. Degradation was 93% after 30 days (ECHA) [Kl. score = 2]. In a Zahn-Wellens test, adipic acid showed 90% degradation after 5 days

(ECHA) [Kl. score = 2]. 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 1.585 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 24.34 L/kg. Based on this value, adipic acid has a low potential for adsorption to soil and sediment and is expected to have very high mobility in soil.

E. Bioaccumulation

No bioconcentration studies have been conducted on adipic acid. Adipic acid is not expected to bioaccumulate based on the experimental $\log K_{ow}$ of 0.093 (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Adipic acid is moderately toxicity to aquatic organisms on an acute and chronic basis.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of the acute aquatic toxicity studies on adipic acid.

Table 3 Acute Aquatic Toxicity Studies on Adipic Acid

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
<i>Danio rerio</i>	96-hour LC_{50}	>1,000	2	ECHA
<i>Leuciscus idus</i>	96-hour LC_{50}	230	2	ECHA
<i>Daphnia magna</i>	48-hour EC_{50}	46	2	ECHA
<i>Daphnia magna</i>	48-hour EC_{50}	85.7	2	ECHA
<i>Pseudokirchnerella subcapitata</i>	72-hour EC_{50}	59	2	ECHA
	72-hour NOEC	41		

Chronic Studies

The NOEC from a 21-day *Daphnia* reproduction study is 6.3 mg/L (ECHA). [Kl. score = 2]

C. Terrestrial Toxicity

No studies are available.

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).

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

The experimental log K_{ow} for adipic acid is 0.093. Thus, adipic acid does not meet the criteria for bioaccumulation.

The NOECs from the chronic aquatic toxicity studies on adipic acid are >0.1 mg/L. The acute EC_{50} values from the acute aquatic toxicity studies on adipic acid are >1 mg/L. Thus, adipic acid does not meet the criteria for toxicity.

The overall conclusion is that adipic acid is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for adipic acid.

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	
Adipic Acid	124-04-9	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

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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/L	grams per litre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kg/m ³	kilogram per cubic metre
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
Pa*m ³ /mol	pascal meter cubed per mol
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	screening information data set
USEPA	United States Environmental Protection Agency