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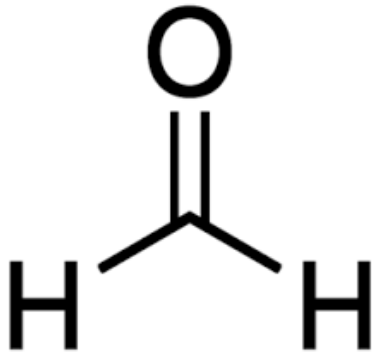
Environmental Protection Agency

March 2024
Office of Chemical Safety and
Pollution Prevention

Draft Chemistry, Fate, and Transport Assessment for Formaldehyde

CASRN 50-00-0



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Key Points: Physical Chemical Properties, Fate, and Transport for Formaldehyde

EPA considered all reasonably available information identified by the Agency through its systematic review process under the Toxic Substances Control Act (TSCA) and submissions under the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) to characterize the physical and chemical properties as well as the fate and transport of formaldehyde. The following bullets summarize the key points of this draft assessment:

- Formaldehyde is a gas that is distributed in a solution as formalin (formaldehyde, methanol, and water) or in a solid as paraformaldehyde. It dissolves quickly in water and reacts with most other chemicals in its environment.
- Due to the reactivity of formaldehyde, it is not expected to be persistent in water and soil, some environmental media but may be abundant due to continual release and formation from secondary sources like organic matter decomposition, combustion, and other chemical releases.
- Formaldehyde is expected to hydrate to methylene glycol in moist soils and react with nucleophiles; however, no confirmatory empirical data are available. In dry soils, formaldehyde is expected to react with nucleophiles, undergo biodegradation by soil microbes (again no confirmatory empirical data are available), or volatilize.
- In water, formaldehyde quickly hydrates to form methylene glycol, which can polymerize to form oligomers of various chain lengths in the absence of methanol. These oligomers or poly(oxy)methylene glycols are susceptible to reactions with nucleophiles to form unknown compounds that would be expected to be structurally dissimilar to formaldehyde and methylene glycol.
- Formaldehyde is susceptible to direct and indirect photolysis in air; however, it may persist in outdoor and indoor air environments with little or no sunlight.
- EPA is confident in the fate and transport characterization of formaldehyde and its transformation products. The greatest uncertainty is associated with the rate of transformation and transport of methylene glycol and poly(oxy)methylene glycols in water and soil.

EXECUTIVE SUMMARY

Formaldehyde is a colorless gas with a high vapor pressure. In air, the half-life of formaldehyde depends greatly on the intensity and duration of sunlight and ambient conditions such as temperature and humidity. Under direct sunlight, formaldehyde will undergo photolysis with a half-life up to 4 hours yielding mainly hydroperoxyl radical (HO_2), carbon monoxide (CO), and hydrogen (H_2). In the absence of sunlight, studies indicate that formaldehyde can persist with a half-life value up to 114 days. In addition, formaldehyde may hydrate in moist air to form methylene glycol and later formic acid. In indoor environments, the persistence of formaldehyde is driven by dissipation and adsorption. Based on this information, formaldehyde is expected to readily transform in outdoor air but may be persistent in indoor air.

Formaldehyde is soluble in water and not expected to volatilize from water. Formaldehyde is often distributed in water and methanol as formalin; methanol is used as a stabilizer to stop polymerization. Formaldehyde can also be distributed as paraformaldehyde in a white crystalline solid form. In aqueous solutions, formaldehyde is expected to rapidly hydrate and exist in equilibrium with methylene glycol and oligomers of various chain lengths—mainly low molecular weight poly(oxy)methylene glycols (n = 1–7) and paraformaldehyde. Therefore, multiple compounds (formaldehyde, methylene glycol,

poly(oxy)methylene glycol, and paraformaldehyde) can occur simultaneously with any introduction of formaldehyde to water, though the methylene glycol form is expected to be dominant. Because dissolved formaldehyde in water is expected to be present in low concentrations (≤0.1 wt%), exposure to formaldehyde in aquatic environments is expected to be low. Little data are available to assess the fate and transport of the identified formaldehyde transformation products in water. However, available data suggest the formaldehyde transformation products are more persistent than formaldehyde but still readily transform in water and/or precipitate out of solution. As such, downstream transport of formaldehyde and closely related transformation products is not expected.

While formaldehyde is not expected to bind to soil, it is expected to undergo abiotic (hydration and nucleophilic addition) chemical reactions in soils, limiting the likelihood it will leach through the soil profile. Formaldehyde may volatilize from soil, especially dry soils. Due to rapid hydration of formaldehyde, methylene glycol might be present in moist soil; however, no information is available on the transformation of methylene glycol in soils.

Taken together, EPA has high confidence in the overall fate and transport profile of formaldehyde and paraformaldehyde; however, EPA is less confident in the overall fate and transport of the transformation products methylene glycol and poly(oxy)methylene glycol.

1 INTRODUCTION

This draft assessment of the physical and chemical properties and the fate and transport of formaldehyde is a joint assessment that will serve as a reference for both the Office of Pesticide Programs (OPP) and the Office of Pollution Prevention and Toxics (OPPT) in EPA's Office of Chemical Safety and Pollution Prevention (OCSPP) as part of their ongoing regulatory efforts. The properties listed in this assessment are based on the best available information may differ from those previously published by OPP and OPPT.

1.1 Risk Evaluation Scope

The TSCA risk evaluation of formaldehyde comprises several human health and environmental assessment modules and two risk assessment documents—the ecological risk assessment and the human health risk assessment. A basic diagram showing the layout of these assessments and their relationships to the Draft Toxic Substances Control Act (TSCA) Risk Evaluation is provided in Figure 1-1. In some cases, modular assessments were completed jointly under TSCA and Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA). These modules are shown in dark gray. This chemistry, fate, and transport module, which is also a shared TSCA/FIFRA assessment, is shaded blue.

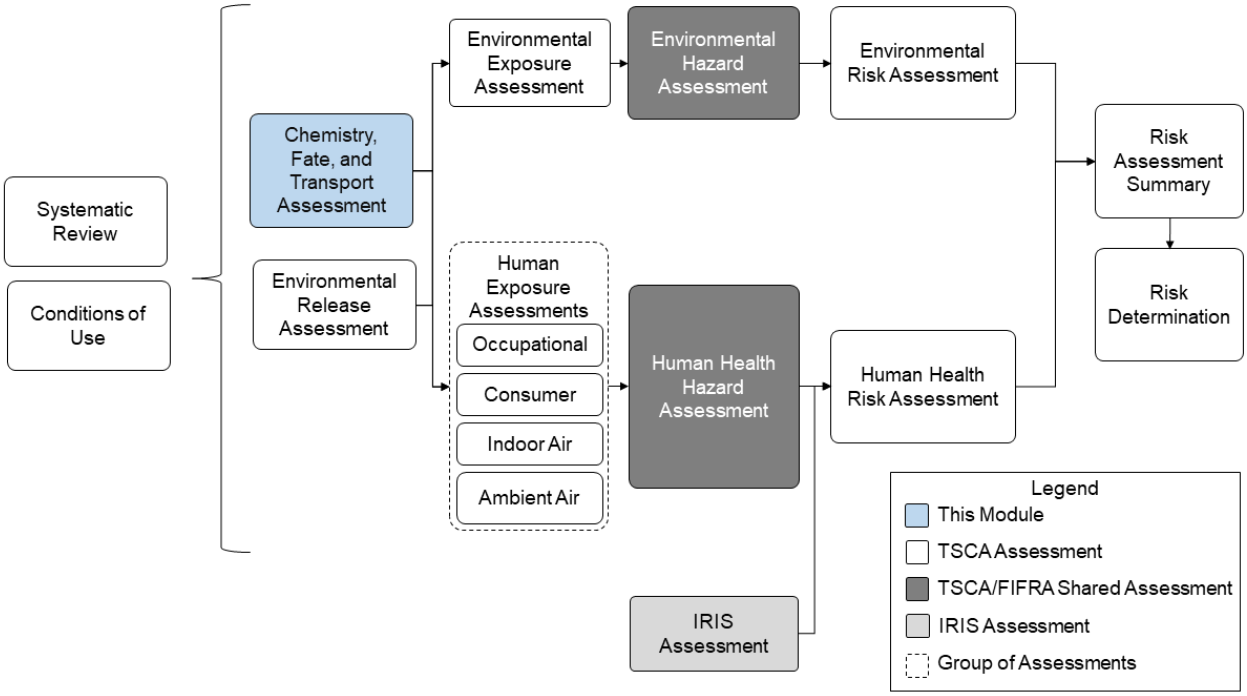

Figure 1-1. Risk Evaluation Document Summary Map

1.2 Approach and Methodology

EPA reviewed the best available data for physical and chemical properties as well as the fate and transport of formaldehyde and its transformation products to better understand how these compounds will behave in various environmental compartments.

The Agency identified chemical and physical properties for formaldehyde, methylene glycol, formalin, and paraformaldehyde based on all data available to OPP and OPPT. Methylene glycol and paraformaldehyde have unique Chemical Abstracts Service (CAS) numbers and may be subject to future

prioritization and risk evaluations under TSCA; due to the unique chemical nature of formaldehyde compounds, the chemicals are presented here to account for the transformation of formaldehyde in the environment.

EPA identified best available environmental transport and fate data, including bioconcentration factors, wastewater treatment, and organic carbon-water partitioning coefficient (K_{OC}). Due to the expansive amount of information available for formaldehyde, EPA selected values from key sources that have been used by other national scale assessments for use in the Risk Evaluation. Example sources considered are provided below:

- Systematic review[1];
- Open literature data;
- EPI Suite™ program v4.11[2] (EPA, 2012a);
- Prior EPA publications such as the *Final Scope of the Risk Evaluation for Formaldehyde CASRN 50-00-0* (EPA, 2020) and OPP's Reregistration Eligibility Determination (EPA, 2008);
- Databases containing publicly available, peer-reviewed literature; and
- Data and information submitted under TSCA sections 4, 5, 8(e), and 8(d) as well as FIFRA.

As much as possible, EPA selected empirical and measured data over modeled data to improve confidence in the endpoints. Other fate estimates were based on modeling results from EPI Suite™, which was reviewed by the EPA Science Advisory Board (SAB, 2007). In addition, the individual models that comprise EPI Suite™ have been peer-reviewed through publication in technical journals. Citations for the supporting manuscripts are available in the EPI Suite™ help files.

Information on the full extracted dataset is available in the supplemental document *Data Extraction of Environmental Fate and Transport Studies for Formaldehyde* (EPA, 2023), while data evaluation information is available in *Data Quality Evaluation of Environmental Fate and Transport Studies for Formaldehyde* (EPA, 2021a).

[1] A full description of the literature searching, search terms, and the Pathways and Processes, Exposure, Setting or Scenario, and Outcomes (PESO) statement can be found in the *Final Scope of the Risk Evaluation for Formaldehyde* (EPA, 2020).
[2] EPI (Estimation Programs Interface) Suite™ is a predictive tool that provides users with estimates of physical/chemical and environmental fate properties. EPI Suite was reviewed by the EPA Science Advisory Board (SAB, 2007) and the individual models that comprise EPI Suite have been peer-reviewed through publication in technical journals. Citations for supporting documents are available in the EPISuite™ help files.

2 PHYSICAL AND CHEMICAL PROPERTIES

Formaldehyde is a colorless gas (vapor pressure of 3,890 mmHg at 25 °C) with a pungent odor (NIOSH, 2007). It is a highly reactive chemical substance that is flammable and readily undergoes polymerization in various media. Formaldehyde is miscible in water, alcohols, and other polar solvents. At low temperatures, liquid formaldehyde is soluble with a wide variety of non-polar organic solvents such as toluene, ether, chloroform, and ethyl acetate.

Formaldehyde is formulated as either a liquid (formalin) or a solid (paraformaldehyde) and this evaluation considers the chemical substance in both forms.

Formalin is a 10 to 50 percent formaldehyde aqueous solution with 0.5 to 15 percent methanol in water. Methanol is added to prevent polymerization to the solid crystalline form. In aqueous solution, formaldehyde exists as methylene glycol with oligomers with chain lengths that can range from 2 to 7 units. This assessment primarily focuses on formalin containing 37 percent formaldehyde, 10 to 15 percent methanol, and water. It is likely that formaldehyde converts to methylene glycol in this solution; however, the extent of this conversion is unknown.

Paraformaldehyde is a white crystalline solid that is the polymerized aldehyde with chain lengths ranging from 8 to 100 units. The number of repeating units affects the physical and chemical properties of the resulting oligomer/polymer. For example, paraformaldehyde molecules with longer chain lengths will have lower vapor pressures and higher melting points.

In aqueous solutions, formaldehyde hydrates to form methylene glycol and can polymerize in the absence of stabilizers like methanol (see Figure 2-1). The equilibrium formation of these oligomers or poly(oxy)methylene glycol depends on formaldehyde concentrations and higher molecular weight oligomers are most prevalent at high concentrations of formaldehyde. However, heat drives the equilibrium toward parent formaldehyde.

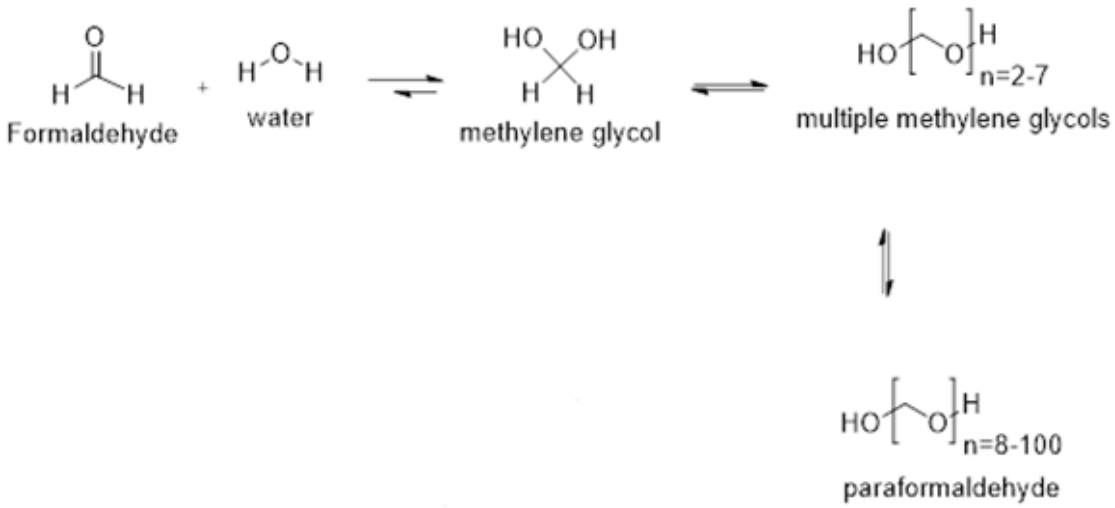

Figure 2-1. Chemical Equilibria for Formaldehyde in Aqueous Solutions
Adapted from (Boyer et al., 2013).

Due to the reactive nature of formaldehyde (and associated transformation products), physical and chemical properties can be difficult to isolate and may imperfectly reflect how the chemical will behave under various conditions. Thus, it is most appropriate to present the physical and chemical

properties of formaldehyde in the gaseous phase as well as in the hydrated forms. Table 2-1 and Table 2-2 summarize the various physical and chemical properties for these compounds and formalin (mixture), respectively.

Table 2-1. Physical and Chemical Properties of Formaldehyde and Transformation Products

Chemical Properties	Formaldehyde	Methylene Glycol	Paraformaldehyde
Molecular formula	CH_2O	$CH_2(OH)_2$	$HO(CH_2O)_nH$ (n = 8–100)
CASRN	50-00-0	463-57-0	30525-89-4
Molecular weight	30.026 g/mol	48.02 g/mol	$(30.03)_n$ g/mol (Varies)
Physical form	Colorless gas	Colorless liquid	White crystalline solid
Melting point	−92.0 to −118.3 °C	−43.8 °C	120 to 170 °C
Boiling point	−19.5 °C	131.6 °C	None identified
Density	0.815 g/cm^3 at 20 °C	1.20 g/cm^3	1.46 g/cm^3 at 15 °C
Vapor pressure	3,890 mmHg at 25 °C	3.11 mmHg at 25°C	1.45 mmHg @ 25 °C
Vapor density	1.067 (air = 1)	None identified	1.03 (air = 1)
Water solubility	<55% 400 to 550 g/L	Miscible	Insoluble
Octanol/water partition coefficient (log K_{OW})	0.35	−0.79	N/A
Henry's Law constant	3.37E−7 atm/m^3·mol at 25 °C	1.65E−7 atm/m^3·mol at 25 °C	N/A
Flash point	N/A	None identified	71.1°C
Autoflammability	300°C	None identified	N/A
Viscosity	1.4E−04 Pa S	None identified	None identified
Refractive index	1.3746	None identified	N/A

[a] Physical and chemical properties for formaldehyde, methylene glycol, formalin, and paraformaldehyde are considered best estimates. Because the chemical substance often exists in a mixture at varying concentrations, these properties can vary based on the equilibration with other chemical substances present.

Table 2-2. Physical and Chemical Properties of Formalin

Chemical Properties	Formalin
Molecular formula	$CH_2O + HO(CH_2O)_nH + H_2O$ (n = 2–7)
CASRN	N/A
Molecular weight	Varies
Physical form	Colorless liquid
Melting point	−15 °C
Boiling point	96 °C
Density	1.083 g/cm^3
Vapor pressure	1.3 mmHg @ 20 °C
Vapor density	None identified
Water solubility	Miscible
Octanol/water partition coefficient (log K_{OW})	None identified
Henry's Law constant	None identified
Flash point	50 to 85 °C
Autoflammability	None identified
Viscosity	None identified
Refractive index	1.3616

Sources of uncertainty in reported physical and chemical property values may include the following:

1. measurement error associated with the instrumental method;
2. precision with which a data point is measured and reported in the data source; and
3. ability of the instrument to differentiate between formaldehyde, its transformation products (methylene glycol and oligomers), or the various chain lengths of those transformation products.

References and data quality ratings for each selected value are provided in Table_Apx A-1, Table_Apx A-2, Table_Apx A-3, and Table_Apx A-4.

3 ENVIRONMENTAL FATE ASSESSMENT

The transport and fate of formaldehyde in the environment depends on the environmental compartment (*i.e.*, outdoor air, surface water, etc.) and is described in the following subsections. Specifically, relevant studies and data are described in more detail within the subsection for the relevant environmental media based on the conceptual exposure model. In each case, best available environmental fate data, removal during wastewater treatment, bioaccumulation data or the lack thereof, and organic carbon:water partition coefficient (log K_{OC}) were used in the current draft risk evaluation to understand how the chemical behaves in various media. When primary data sources were unavailable, EPA selected values based on studies that had been identified and reviewed in other national and international risk assessments.

Figure 3-1 illustrates the transport and partitioning of anthropogenic sources of formaldehyde and its abiotic transformations in the environment. The diagram depicts the distribution (gray arrows) as well as the transport and partitioning (black arrows) of formaldehyde in the environment. The width of the arrow is a qualitative indication that partitioning will occur (*i.e.*, wider arrows suggest likelier partitioning). For formaldehyde, primary sources of transport come from industrial sources either through emissions to air or release to wastewater facilities. Subsequently, the chemical may undergo several transformations to form either methylene glycol, formic acid, or paraformaldehyde, depending on the media. Table 3-1 provides selected environmental fate data for formaldehyde. The data in Table 3-1 were updated after publication of *Final Scope of the Risk Evaluation for Formaldehyde CASRN 50-00-0* (EPA, 2020), with additional information identified through the systematic review process and data submitted to OCSPP under TSCA and FIFRA. Additional information was derived using EPISuite™ and those results are available in Appendix B.

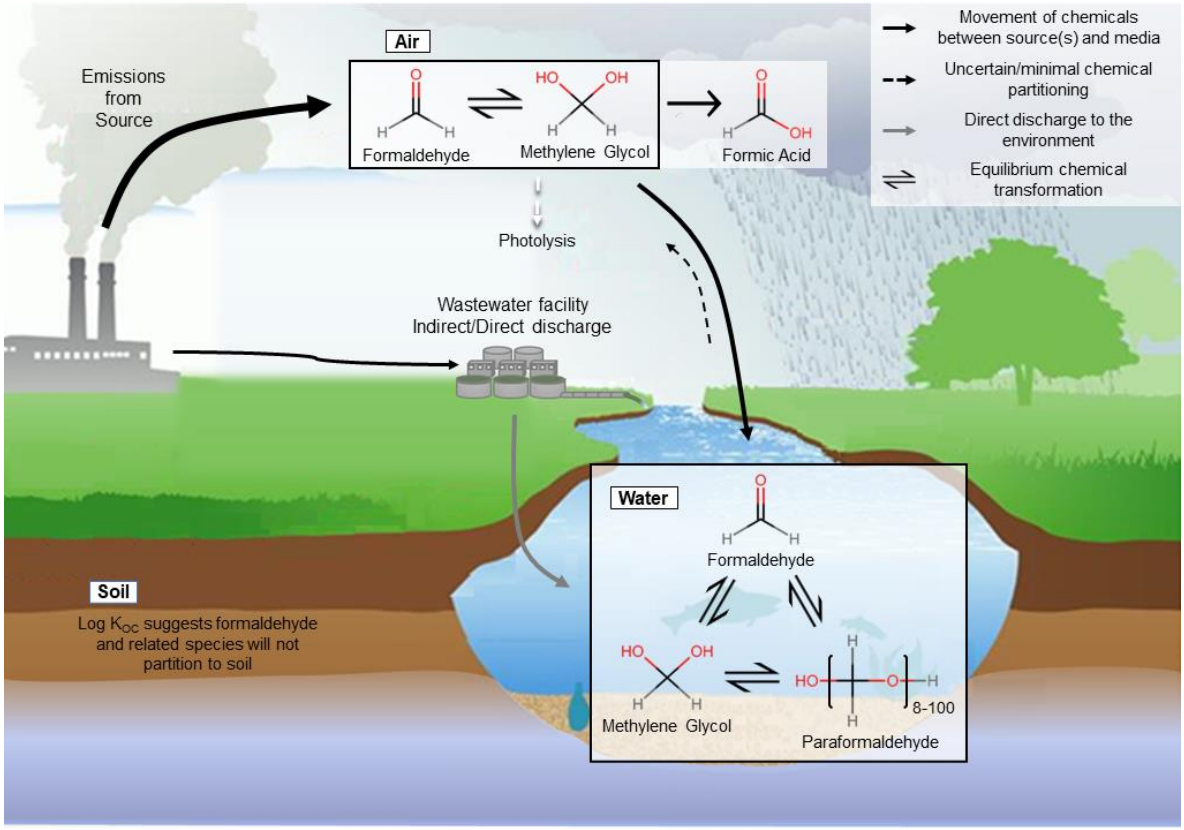

Figure 3-1. Transport and Partitioning of Anthropogenic Sources of Formaldehyde and Abiotic Transformations in the Environment

Table 3-1. Formaldehyde Environmental Fate Properties

Property or Endpoint	Value[a] [b]	Reference(s)	Data Quality Rating
Indirect photodegradation	45 hours (based on $^{-}$OH reaction rate constant 8.5E−12 cm^3/molecule-second at 25 °C) 57 days (based on nitrate radicals reaction rate constant 5.6E−16 cm^3/molecule-second at 25 °C)	(NLM, 2019)	Medium
Direct photodegradation	$t_{1/2}$ = 1.4 to 4 hours in sunlight	(NLM, 2019)	Medium
Hydrolysis half-life	Not expected; however, in an aqueous environment formaldehyde will be fully hydrated to methylene glycol	(OECD, 2002)	Medium
Aerobic aquatic biodegradation	In water from stagnant lake, formaldehyde completely decomposed in ~30 hours under aerobic conditions, 20 °C	(NLM, 2019)	Medium
	In surface water, estimated half-lives of 24 to 168 hours (1–7 days)	(EPA, 2008)	Medium
Anaerobic Aquatic biodegradation	In water from stagnant lake, formaldehyde completely decomposed in ~48 hours under anaerobic conditions, 20 °C	(NLM, 2019)	Medium
Aerobic soil biodegradation	In soil, estimated half-lives of 24 to 168 hours (1–7 days)	(Howard et al., 1991)	Not rated
Bioconcentration factor (BCF)	Based on log K_{OW} <3, potential for bioconcentration in aquatic organisms is considered low	(NLM, 2019; EPA, 2012b)	Medium
	Experiments performed on a variety of fish and shrimp show no bioconcentration of formaldehyde	(Canada, 2000)	Medium
Bioaccumulation factor (BAF)	None identified		
Organic carbon:water partition coefficient (log K_{OC})	1.57 (K_{OC} of 37 L/kg) Formaldehyde not expected to sorb to suspended solids and sediment	(EPA, 2008)	Medium
Wastewater treatment	Removal/secondary treatment: 57 to 99% removal percentages based upon data from a semi-continuous sewage and continuous activated sludge biological treatment simulator	(Howard et al., 1991)	Not rated
	94% total removal (93% by biodegradation)[b]	(EPA, 2012b)	Not rated

[a] Measured unless otherwise noted.
[b] Information estimated using EPISuite™ (EPA, 2012b). Results available in Appendix B.

3.1 Outdoor Air

Formaldehyde can be generated in the air compartment through several natural and anthropogenic processes. Like other volatile organic compounds (VOCs), formaldehyde is a product of physiological and plant-atmosphere exchange processes, including the following:

1. oxidation of methane or methanol in the presence of a catalyst (Atkinson, 2000),
2. decomposition of lignin which is naturally found in most plants (Salthammer et al., 2010), or
3. degradation of isoprenes that are normally found in forested areas.

Formaldehyde in outdoor air is also attributed to activities like industrial releases, fuel combustion, and incineration. Similarly, formaldehyde may be present in the atmosphere due to latent releases from consumer and commercial products and the associated waste streams (NLM, 2019; OECD, 2002). Due to these many types of releases, formaldehyde may appear to be persistent despite having several degradation pathways in air.

In outdoor air, formaldehyde degrades primarily through direct and indirect photolysis yielding mainly hydroperoxyl radical (HO_2), carbon monoxide (CO), and hydrogen (H_2). Additionally, formaldehyde may be removed from the air through dry deposition or wet deposition after transfer into rain, fog, or clouds (NLM, 2019; Dąbrowska and Nawrocki, 2013). In these latter compartments, formaldehyde is expected to convert to methylene glycol or formic acid. These compounds have much lower vapor pressures and therefore are less likely to remain in air compared to formaldehyde. Methylene glycol or formic acid have been detected in rainwater where local emissions of formaldehyde are high (Franco et al., 2021).

Reaction with hydroxyl radicals (HO·) and direct photolysis is the major transformation route for gas-phase formaldehyde (NLM, 2019). Hydroxyl radical concentrations vary as a function of time of day, sunlight intensity, and temperature (Salthammer et al., 2010). However, because hydroxyl radicals are short-lived in the atmosphere, the radicals are only prevalent at significant concentrations during daylight (Stone et al., 2012). Consequently, the reaction of formaldehyde via indirect photolysis is expected to be limited at night. Overall, the atmospheric half-life of formaldehyde, based on the hydroxyl radical rate constant and concentrations, is expected to be between 1.24 (Salthammer et al., 2010) and 1.88 days (NLM, 2019). Formaldehyde also absorbs ultraviolet radiation at wavelengths of greater than 360 nm and therefore is expected to be subject to direct photolysis by sunlight, with a half-life on the order of 1 to 4 hours (NLM, 2019).

Formaldehyde also reacts with nitrate radicals in the outdoor air. Unlike the hydroxyl radical, the nitrate radical undergoes rapid direct photolysis and is not present in high concentrations during daylight. Therefore, the reaction between formaldehyde and the nitrate radical occurs primarily during the night (Canada, 2000). Nighttime concentrations are often higher near cities and industrial centers, and an order of magnitude lower near rural areas (Atkinson et al., 1986). Data also indicate that formaldehyde concentrations tend to be lower at higher elevations where the atmospheric concentration of nitrate radical is lower. Sea-level concentrations, combined with a reaction rate of 5.60×10^{-16} cm^3 $molecule^{-1}$ s^{-1} (NLM, 2019; Feilberg et al., 2004; Hellen et al., 2004) result in formaldehyde half-live values of 11.4 and 114 days (assuming 12 hours of daylight per day) for urban and rural areas, respectively.

The slowest atmospheric reaction of formaldehyde is with ozone. The half-life value for this reaction is greater than 4.5 years (Salthammer et al., 2010); therefore, it is not expected to be a relevant transformation route for formaldehyde.

3.2 Indoor Air

EPA did not intentionally gather or evaluate data and information on the indoor fate of formaldehyde according to the process described in the *Draft Systematic Review Protocol Supporting TSCA Risk Evaluations for Chemical Substances* (EPA, 2021b). Instead, EPA searched for articles available via

Google Scholar using keywords to describe the fate and transport of formaldehyde in the indoor environment.

Formaldehyde is not subject to the various transformation and degradation processes in the indoor air environment that are expected in the outdoor environment (Salthammer et al., 2010). Thus, its persistence is driven by dissipation and adsorption. The major route of dissipation of formaldehyde in the indoor environments is by mechanical removal via ventilation systems. Adsorption of formaldehyde to surfaces may occur based on the surfaces composition; however, it may re-emit at warmer temperatures (Plaisance et al., 2013; Cousins, 2012; Traynor et al., 1982).

3.3 Surface Water and Sediments

In the presence of water, formaldehyde hydrates rapidly to methylene glycol, with a 50 percent conversion rate in 65 milliseconds and a 90 percent conversion rate in 215 milliseconds at 298K (25 °C, based on rate constants) (Winkelman et al., 2002). Limited data are available on the fate and transport of methylene glycol; however, as previously mentioned, it has been detected in rainwater in areas of high formaldehyde concentrations.

Methylene glycol is expected to transform to oligomers ($HO(CH_2O)_nH$) in the presence of low concentrations of formaldehyde and polymerizes to paraformaldehyde in concentrated solutions of formaldehyde. The equilibria transformation of monomeric formaldehyde to methylene glycol occurs within seconds while the formation of the corresponding oligomers or poly(oxy)methylene glycol occurs within minutes. The formation of paraformaldehyde takes hours to days (Commission, 2012). This polymerization is expected to occur faster at higher formaldehyde concentrations and thus under typical environmental conditions is likely to occur slowly or not at all. The poly(oxy)methylene glycol reactions with nucleophiles are expected to occur quicker than polymerization, therefore, limiting the formation of paraformaldehyde in the environment (Commission, 2012). As such, poly(oxy)methylene glycol is expected to be the primary residue found in aquatic environmental and these compounds are expected to readily react with nucleophiles to form unidentified compounds that are expected to structurally dissimilar to formaldehyde and methylene glycol.

In aerobic aquatic environments, the complete decomposition of formaldehyde in water from a stagnant lake was estimated to be approximately 30 hours at 20 °C (NLM, 2019), while half-lives in surface water have been estimated at between 1 and 7 days (EPA, 2008; Howard et al., 1991). There is uncertainty in these half-life estimates as the necessary information was not provided including the composition of the test material and the study did not measure concentrations of formaldehyde or its known transformation products. In an anaerobic environment, the complete decomposition of formaldehyde in surface water from a stagnant lake was estimated to be approximately 48 hours at 20 °C (NLM, 2019).

If formed, because paraformaldehyde is insoluble in water it will precipitate. Formaldehyde might undergo similar abiotic chemical reactions in sediments and is not expected to sorb to sediments, based on a log K_{OC} value of 1.57 (EPA, 2008).

3.4 Bioaccumulation and Bioconcentration

Formaldehyde has a log K_{OW} of 0.35, therefore bioconcentration potential is low (NLM, 2019). Methylene glycol has an estimated log K_{OW} of −0.79, similarly confirming low bioconcentration (EPA, 2012a). Other assessments have considered data for fish and shrimp but have also indicated no bioconcentration (*e.g.*, (Canada, 2000)).

3.5 Soils

Formaldehyde can be formed in the early stages of plant residue decomposition in soil and is reportedly degraded by bacteria in the soil; however, there are no available data to confirm this assumption or identify transformation products. In aerobic soil, half-lives have been estimated at between 1 and 7 days based on aqueous aerobic biodegradation (Howard et al., 1991).

Based on an empirical Henry's Law constant of 3.37×10^{-7} atm-m^3/mol at 25 °C (NLM, 2019), formaldehyde can volatilize slowly from moist soil. In dry soil, formaldehyde is expected to volatilize more rapidly. Due to rapid hydration of formaldehyde in moist soil, methylene glycol is expected to be present. However, no data are available on the transformation of methylene glycol in soil.

3.6 Groundwater

As described in the Surface Water and Sediments section, formaldehyde, and its transformation products are challenging to characterize in water including groundwater; however, it may be present from the microbially-mediated breakdown of other organic compounds. In groundwater, estimated formaldehyde half-lives range from 48 to 336 hours (2 to 14 days) (EPA, 2008; Howard et al., 1991). There is uncertainty in these half-life estimates as the necessary information was not provided including the composition of the test material and the study did not measure concentrations of formaldehyde or its known transformation products.

3.7 Wastewater Treatment and Biosolids

3.7.1 Wastewater Treatment

Biological wastewater treatment systems have shown a mean removal of 99.9 percent when concentrations of formaldehyde are 2,087 to 2,200 mg/L (Eiroa et al., 2006). Some of this removal is due to transformation of the chemical into formic acid. When evaluated at different stages of treatment, the aerobic phase of treatment was demonstrated to be one of the most effective processes at removing formaldehyde (Garrido et al., 2000). EPI Suite™ suggests that when formaldehyde is modeled using the STPWIN™, formaldehyde may be removed with 94 percent efficiency. Of this, 93 percent of the removal can be attributed to biodegradation (EPA, 2012b); See Appendix B.1. A removal efficiency of between 57 to 99 percent based on data from a semi-continuous sewage and continuous activated sludge biological treatment simulator has also been reported (Howard et al., 1991). Taken together, these data indicate formaldehyde is not expected to be present in water following treatment.

3.7.2 Biosolids

Due to its removal via biodegradation and aerobic phases (see Table 3-1 and Appendix B.1), EPA does not anticipate residues of formaldehyde to be present in biosolids because of releases of formaldehyde to a wastewater facility. It may, however, be present due to the degradation of other organic compounds.

3.8 Strengths, Limitations, Assumptions, and Key Sources of Uncertainty for the Fate and Transport Assessment

EPA has high confidence in the overall fate and transport profile of formaldehyde and paraformaldehyde; however, EPA is less confident in the overall fate and transport of the transformation products methylene glycol and poly(oxy)methylene glycol. Key sources of uncertainty for this assessment are related to formaldehyde's equilibrium in various media and subsequent transformation. As previously mentioned, formaldehyde quickly forms methylene glycol and poly(oxy)methylene glycol in aqueous media and its transport is difficult to characterize with high certainty. Similarly, the natural formation and abundance of formaldehyde may suggest that the chemical substance persists for longer

than expected given its reactivity. In cases where there is little or fate and transport data, EPA relied on physical and chemical properties to describe the expected fate and transport of the respective chemical. As such, while EPA has some uncertainty in the precision of a specific parameter value, it has confidence in the overall fate and transport profile of formaldehyde.

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APPENDICES

Appendix A PHYSICAL AND CHEMICAL PROPERTIES AND FATE AND TRANSPORT DETAILS

A.1 Physical and Chemical Properties Evidence Integration

The physical and chemical property values selected for use in the risk evaluation for formaldehyde, its transformation products, and formalin are provided in Table 2-1 and Table 2-2. These values were taken from the *Final Scope of the Risk Evaluation for Formaldehyde CASRN 50-00-0* (EPA, 2020), except for values identified for methylene glycol, paraformaldehyde, and formalin. In some cases, higher quality endpoints could be identified and were selected for use in the risk evaluation. All data quality ratings for each substance can be found in Table_Apx A-1 through Table_Apx A-4.

Table_Apx A-1. References and Data Quality Ratings for the Physical and Chemical Properties of Formaldehyde

Property	Selected Value(s) [a] [b]	Reference(s)	Data Quality Rating
Molecular formula	CH_2O	N/A	
Molecular weight	30.026 g/mol	N/A	
Physical form	Colorless gas	(NIOSH, 2007)	High
Melting point	−92.0 to −118.3 °C	(Elsevier, 2019)	High
Boiling point	−19.5 °C	(O'Neil, 2013)	High
Density	0.815 g/cm^3 at 20 °C	(Rumble, 2018)	High
Vapor pressure	3,890 mmHg at 25 °C	(NLM, 2019)	High
Vapor density	1.067 (air = 1)	(NLM, 2019)	High
Water solubility	<55% 400 to 550 g/L	(O'Neil, 2013), (Canada, 2000)	High
Octanol/water partition coefficient (log K_{OW})	0.35	(NLM, 2019)	High
Henry's Law constant	3.37E−07 atm/m^3 at 25 °C	(NLM, 2019)	High
Flash point	N/A[c]		
Autoflammability	300 °C	(O'Neil, 2013)	High
Viscosity	1.4E−04 Pa S	(NLM, 2019)	High
Refractive index	1.3746	(NLM, 2019)	High

[a] Care should be taking in interpreting or using reported values due to polymerization of the chemical substance
[b] Measured unless otherwise noted
[c] Value only available for formalin

Table_Apx A-2. References and Data Quality Ratings for the Physical and Chemical Properties of Methylene Glycol

Property	Selected Value(s) [a]	Reference(s)	Data Quality Rating
Molecular formula	$CH_2(OH)_2$	N/A	N/A
Molecular weight	48.02 g/mol	N/A	N/A
Physical form	None identified		N/A
Melting point	−43.8 °C	(EPA, 2012a)	
Boiling point	131.6 °C	(EPA, 2012a)	N/A
Density	1.2 g/cm^3 [b]	(RSC, 2019)	Medium
Vapor pressure	3.11 mmHg at 25 °C	(EPA, 2012a)	N/A
Vapor density	None identified		N/A
Water solubility	Miscible	(EPA, 2012a)	N/A
Octanol/water partition coefficient (log K_{ow})	−0.79	(EPA, 2012a)	N/A
Henry's Law constant	1.65E−07 atm/m^3 at 25 °C [b]	(Meylan and Howard, 1991)	High
Flash point	99.8 °C [b]	(RSC, 2019)	Medium
Autoflammability	None identified		N/A
Viscosity	None identified		N/A
Refractive index	None identified		N/A

[a] Calculated using EpiSuite™ unless otherwise noted with an asterisk. See Appendix B for full output.
[b] Modeled value

Table_Apx A-3. References and Data Quality Ratings for the Physical and Chemical Properties of Formalin (37% Formaldehyde; 6–15%, and Water)

Property	Selected Value(s) [a]	Reference(s)	Data Quality Rating
Molecular formula	CH_2O + $HO(CH_2O)_nH$ + H_2O (n = 2–7)		N/A
Molecular weight	Varies	(NIOSH, 2007)	High
Physical form	Colorless liquid with a pungent irritating odor	(NLM, 2019)	High
Melting point	−15 °C	(NIOSH, 1988a)	Medium
Boiling point	96 °C	(O'Neil, 2013)	High
Density	1.083g/L at 20 °C	(RSC, 2019)	Medium
Vapor pressure	1.3 mmHg at 20 °C	(EPA, 2008)	Medium
Vapor density	None identified		N/A
Water solubility	Miscible	(NLM, 2019)	High
Octanol/water partition coefficient (log K_{OW})	N/A	N/A	N/A
Henry's Law constant	None identified		N/A
Flash point	50 to 85 °C	(NLM, 2019)	High
Autoflammability	430 °C	(NIOSH, 1988b)	Medium
Viscosity	2.05E−04 Pa S	(Winkelman and Beenackers, 2000)	High
Refractive index	1.3616	(Saunders et al., 2016)	High
[a] Measured unless otherwise noted			

Table_Apx A-4. References and Data Quality Ratings for the Physical and Chemical Properties of Paraformaldehyde

Property	Selected Value(s) [a]	Reference(s)	Data Quality Rating
Molecular formula	$HO(CH_2O)_nH$ (n = 8–100)	N/A	N/A
Molecular weight	$(30.03)_n$ g/mol (varies)	N/A	N/A
Physical form	White crystalline solid	(NLM, 2019)	High
Melting point	120 to 170 °C	(EPA, 2008)	Medium
Boiling point	None identified		N/A
Density	1.46 g/cm^3 at 15 °C	(EPA, 2008)	Medium
Vapor pressure	1.45 mmHg @ 25 °C	(EPA, 2008)	Medium
Vapor density	1.03 (air = 1)	(NCBI, 2020)	Medium
Water solubility	Insoluble	(NLM, 2019)	High
Octanol/water partition coefficient (log K_{OW})	None identified		N/A
Henry's Law constant	None identified		N/A
Flash point	71.1 °C	(NCBI, 2020)	Medium
Autoflammability	None identified		N/A
Viscosity	None identified		N/A
Refractive index	None identified		N/A

[a] Measured unless otherwise noted

A.2 Fate and Transport Properties Evidence Integration

The fate and transport property values selected for use in the risk evaluation for formaldehyde are given in Table 3-1. These values were taken from the *Final Scope of the Risk Evaluation for Formaldehyde CASRN 50-00-0* (EPA, 2020) except for direct photolysis, aerobic biodegradation rates, bioaccumulation factors, and the organic carbon:water partition coefficient.

Appendix B EPISuite™ Results

To set up EPI Suite™ for estimating fate properties of formaldehyde and its transformation products, the physical and chemical properties were input based on the values in Table 2-1. When there was uncertainty around which value to select, EPI Suite™ was run using default settings (*i.e.*, no other parameters were changed or input). The results are shown below in Appendices B.1 and B.2.

B.1 EPISuite™ Results for Formaldehyde

SMILES: O=C
CHEM: Formaldehyde
MOL FOR: C1 H2 O1
MOL WT: 30.03
---------- EPI SUMMARY (v4.11) ----------
Physical Property Inputs:
Log Kow (octanol-water): 0.35
Boiling Point (deg C): -19.50
Melting Point (deg C): -92.00
Vapor Pressure (mm Hg): 3890
Water Solubility (mg/L): 5.5E+005
Henry LC (atm-m3/mole): 3.37E-007

KOWWIN Program (v1.68) Results:
==========

Log Kow(version 1.68 estimate): 0.35

Experimental Database Structure Match:
Name: FORMALDEHYDE
CAS Num: 000050-00-0
Exp Log P: 0.35
Exp Ref: HANSCH,C ET AL. (1995)

SMILES: O=C
CHEM: Formaldehyde
MOL FOR: C1 H2 O1
MOL WT: 30.03

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Formaldehyde experimental value - constant	0.1210	0.1210
Const		Equation Constant		0.2290

Log Kow = 0.3500

MPBPVP (v1.43) Program Results:
==========
Experimental Database Structure Match:
Name: FORMALDEHYDE
CAS Num: 000050-00-0
Exp MP (deg C): -92
Exp BP (deg C): -19.1
Exp VP (mm Hg): 3.89E+03 (extrapolated)
(Pa): 5.19E+005
Exp VP (deg C): 25
Exp VP ref: BOUBLIK,T ET AL. (1984)

SMILES: O=C
CHEM: Formaldehyde
MOL FOR: C1 H2 O1
MOL WT: 30.03
---------- SUMMARY MPBVP v1.43 ----------

Boiling Point: 9.50 deg C (Adapted Stein and Brown Method)

Melting Point: -113.76 deg C (Adapted Joback Method)
Melting Point: -108.11 deg C (Gold and Ogle Method)
Mean Melt Pt: -110.94 deg C (Joback; Gold,Ogle Methods)
Selected MP: -110.94 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: -19.50 deg C (user entered))
(MP not used for liquids)
VP: 3.72E+003 mm Hg (Antoine Method)
VP: 4.96E+005 Pa (Antoine Method)
VP: 3.35E+003 mm Hg (Modified Grain Method)
VP: 4.46E+005 Pa (Modified Grain Method)
VP: 3.03E+003 mm Hg (Mackay Method)
VP: 4.04E+005 Pa (Mackay Method)
Selected VP: 3.54E+003 mm Hg (Mean of Antoine & Grain methods)
VP: 4.71E+005 Pa (Mean of Antoine & Grain methods)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CHO (aldehyde)	83.38	83.38
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		281.56
RESULT- corr		BOILING POINT in deg Kelvin		282.66
		BOILING POINT in deg C		9.50

TYPE | NUM | MELT DESCRIPTION | COEFF | VALUE
-------+-----+-------------------+----------+---------
Group | 1 | -CHO (aldehyde) | 36.90 | 36.90
* | | Equation Constant | | 122.50
=============+====================+==========+=========
RESULT | MELTING POINT in deg Kelvin | 159.40
| MELTING POINT in deg C | -113.76

Water Sol from Kow (WSKOW v1.42) Results:
==========

Water Sol: 5.498e+004 mg/L

Experimental Water Solubility Database Match:
Name: FORMALDEHYDE
CAS Num: 000050-00-0
Exp WSol: 4E+005 mg/L (20 deg C)
Exp Ref: PICKRELL,JA ET AL. (1983)

SMILES: O=C
CHEM: Formaldehyde
MOL FOR: C1 H2 O1
MOL WT: 30.03

---------- WSKOW v1.42 Results ----------

Log Kow (estimated): 0.35
Log Kow (experimental): 0.35
Cas No: 000050-00-0
Name: FORMALDEHYDE
Refer: HANSCH,C ET AL. (1995)
Log Kow used by Water solubility estimates: 0.35 (user entered)

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction

Melting Pt (Tm) = -92.00 deg C (Use Tm = 25 for all liquids)

Correction(s): Value
---------- -----
No Applicable Correction Factors

Log Water Solubility (in moles/L): 0.263
Water Solubility at 25 deg C (mg/L): 5.498e+004

WATERNT Program (v1.01) Results:
==========

Water Sol (v1.01 est): 3.9694e+005 mg/L

Experimental Water Solubility Database Match:
Name: FORMALDEHYDE
CAS Num: 000050-00-0
Exp WSol: 4E+005 mg/L (20 deg C)
Exp Ref: PICKRELL,JA ET AL. (1983)

SMILES: O=C
CHEM: Formaldehyde
MOL FOR: C1 H2 O1
MOL WT: 30.03

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Formaldehyde experimental value - constant	0.8720	0.8720
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = 1.1212
Water Solubility (mg/L) at 25 dec C =3.9694e+005

ECOSAR Program (v1.11) Results:
==========
ECOSAR Version 1.11 Results Page

SMILES: O=C
CHEM: Formaldehyde
CAS Num:
ChemID1:
MOL FOR: C1 H2 O1
MOL WT: 30.03
Log Kow: 0.350 (EPISuite Kowwin v1.68 Estimate)
Log Kow: (User Entered)
Log Kow: 0.35 (PhysProp DB exp value - for comparison only)
Melt Pt: -92.00 (deg C, User Entered for Wat Sol estimate)
Melt Pt: -92.00 (deg C, PhysProp DB exp value for Wat Sol est)
Wat Sol: 5.498E+004 (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol: 5.5E+005 (mg/L, User Entered)
Wat Sol: 4E+005 (mg/L, PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log Kow: 0.350 (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 5.5E+005 (mg/L, User Entered)

ECOSAR v1.11 Class-specific Estimations

Aldehydes (Mono)

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Aldehydes (Mono)	: Fish	96-hr	LC50	12.544
Aldehydes (Mono)	: Daphnid	48-hr	LC50	46.086
Aldehydes (Mono)	: Green Algae	96-hr	EC50	48.403
Aldehydes (Mono)	: Fish		ChV	3.636
Aldehydes (Mono)	: Daphnid		ChV	4.923 !
Aldehydes (Mono)	: Green Algae		ChV	12.182
Aldehydes (Mono)	: Fish (SW)	96-hr	LC50	17.899
Aldehydes (Mono)	: Fish (SW)		ChV	1.652 !
Neutral Organic SAR (Baseline Toxicity)	: Fish	96-hr	LC50	748.117
	: Daphnid	48-hr	LC50	364.758
	: Green Algae	96-hr	EC50	144.722
	: Fish		ChV	61.098
	: Daphnid		ChV	23.279
	: Green Algae		ChV	26.995

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

NOTE: ! = exclamation designates: The toxicity value was estimated through application of acute-to-chronic ratios per methods outlined in the ECOSAR Methodology Document provided in the ECOSAR Help Menu.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Aldehydes (Mono):

Maximum LogKow: 5.0 (LC50)
Maximum LogKow: 6.4 (EC50)
Maximum LogKow: 8.0 (ChV)

Baseline Toxicity SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)

Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)

HENRYWIN (v3.20) Program Results:
==========
Bond Est: 9.29E-005 atm-m3/mole (9.41E+000 Pa-m3/mole)
Group Est: 6.14E-005 atm-m3/mole (6.23E+000 Pa-m3/mole)

SMILES: O=C
CHEM: Formaldehyde
MOL FOR: C1 H2 O1
MOL WT: 30.03
---------- HENRYWIN v3.20 Results ----------

Experimental Database Structure Match:
Name: FORMALDEHYDE
CAS Num: 000050-00-0
Exp HLC: 3.37E-07 atm-m3/mole (0.0341 Pa-m3/mole)
Temper: 25 deg C
Exp Ref: BETTERTON,EA & HOFFMAN,MR (1988)

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	2 Hydrogen to Carbonyl (C=O) Bonds		2.4206
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	2.421

HENRYs LAW CONSTANT at 25 deg C = 9.29E-005 atm-m3/mole
= 3.80E-003 unitless
= 9.41E+000 Pa-m3/mole

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	1 H2CO	EXPERIMENTAL	2.60
RESULT	GROUP ESTIMATION METHOD for LOG GAMMA VALUE	TOTAL	2.60

HENRYs LAW CONSTANT at 25 deg C = 6.14E-005 atm-m3/mole
= 2.51E-003 unitless
= 6.23E+000 Pa-m3/mole

For Henry LC Comparison Purposes:
Exper Database: 3.37E-07 atm-m3/mole (3.41E-002 Pa-m3/mole)
User-Entered Henry LC: 3.370E-007 atm-m3/mole (3.415E-002 Pa-m3/mole)

Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 5.460E-005 atm-m3/mole (5.532E+000 Pa-m3/mole)
VP: 3.89E+003 mm Hg (source: User-Entered)
WS: 5.5E+005 mg/L (source: User-Entered)

Log Octanol-Air (KOAWIN v1.10) Results:
==========
Log Koa: 5.211

SMILES: O=C
CHEM: Formaldehyde
MOL FOR: C1 H2 O1
MOL WT: 30.03
---------- KOAWIN v1.10 Results ----------

Log Koa (octanol/air) estimate: 5.211
Koa (octanol/air) estimate: 1.625e+005
Using:
Log Kow: 0.35 (user entered)
HenryLC: 3.37e-007 atm-m3/mole (user entered)
Log Kaw: -4.861 (air/water part.coef.)

LogKow: 0.35 (exp database)
LogKow: 0.35 (KowWin estimate)
Henry LC: 3.37e-007 atm-m3/mole (exp database)
Henry LC: 9.29e-005 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate: 2.770 (from KowWin/HenryWin)

BIOWIN (v4.10) Program Results:
==========
SMILES: O=C
CHEM: Formaldehyde
MOL FOR: C1 H2 O1
MOL WT: 30.03
---------- BIOWIN v4.10 Results ----------
Biowin1 (Linear Model Prediction): Biodegrades Fast
Biowin2 (Non-Linear Model Prediction): Biodegrades Fast
Biowin3 (Ultimate Biodegradation Timeframe): Weeks
Biowin4 (Primary Biodegradation Timeframe): Days
Biowin5 (MITI Linear Model Prediction): Biodegrades Fast
Biowin6 (MITI Non-Linear Model Prediction): Biodegrades Fast
Biowin7 (Anaerobic Model Prediction): Biodegrades Fast
Ready Biodegradability Prediction: YES

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aldehyde [-CHO]	0.2846	0.2846
MolWt	*	Molecular Weight Parameter		-0.0143
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		1.0179

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aldehyde [-CHO]	7.1804	7.1804
MolWt	*	Molecular Weight Parameter		-0.4264
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.9999

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aldehyde [-CHO]	0.0223	0.0223
MolWt	*	Molecular Weight Parameter		-0.0664
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		3.1551

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aldehyde [-CHO]	0.1966	0.1966
MolWt	*	Molecular Weight Parameter		-0.0433
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		4.0011

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aldehyde [-CHO]	0.4114	0.4114
MolWt	*	Molecular Weight Parameter		-0.0893
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		1.0342

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aldehyde [-CHO]	2.7436	2.7436
MolWt	*	Molecular Weight Parameter		-0.8668
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.9879

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aldehyde [-CHO]	0.1226	0.1226
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		0.9587

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast
Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then

the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

BioHCwin (v1.01) Program Results:
==========
SMILES: O=C
CHEM: Formaldehyde
MOL FOR: C1 H2 O1
MOL WT: 30.03

---------- BioHCwin v1.01 Results ----------
NO Estimate Possible ... Structure NOT a Hydrocarbon
(Contains atoms other than C, H or S (-S-))

AEROWIN Program (v1.00) Results:
==========
Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 5.19E+005 Pa (3.89E+003 mm Hg)
Log Koa (Koawin est): 5.211
Kp (particle/gas partition coef. (m3/ug)):
Mackay model: 5.78E-012
Octanol/air (Koa) model: 3.99E-008
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model: 2.09E-010
Mackay model: 4.63E-010
Octanol/air (Koa) model: 3.19E-006

AOP Program (v1.92) Results:
==========
SMILES: O=C
CHEM: Formaldehyde
MOL FOR: C1 H2 O1
MOL WT: 30.03

---------- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) --------
Hydrogen Abstraction = 8.1300 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec

Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 8.1300 E-12 cm3/molecule-sec
HALF-LIFE = 1.316 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 15.787 Hrs
---------- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database Structure Match:
Chem Name: Formaldehyde
CAS Number: 000050-00-0
Exper OH rate constant: 9.37 E-12 cm3/molecule-sec
Exper OH Reference: KWOK,ESC & ATKINSON,R (1994)
Exper Ozone rate constant: 2.1 E-24 cm3/molecule-sec
Exper NO3 rate constant: 5.8 E-16 cm3/molecule-sec
Fraction sorbed to airborne particulates (phi):
3.36E-010 (Junge-Pankow, Mackay avg)
3.19E-006 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

KOCWIN Program (v2.00) Results:
==========
SMILES: O=C
CHEM: Formaldehyde
MOL FOR: C1 H2 O1
MOL WT: 30.03
---------- KOCWIN v2.00 Results ----------

Koc Estimate from MCI:

First Order Molecular Connectivity Index ..... : 1.000
Non-Corrected Log Koc (0.5213 MCI + 0.60) ..... : 1.1211
Fragment Correction(s):
1 Misc (C=O) Group (aliphatic attach).... : -1.6047
Corrected Log Koc ..... : -0.4836
Over Correction Adjustment to Lower Limit Log Koc ... : 0.0000

Estimated Koc: 1 L/kg <==========

Koc Estimate from Log Kow:

Log Kow (User entered) ..... : 0.35
Non-Corrected Log Koc (0.55313 logKow + 0.9251) .... : 1.1187
Fragment Correction(s):
1 Misc (C=O) Group (aliphatic attach).... : -0.2293

Corrected Log Koc ..... : 0.8894

Estimated Koc: 7.752 L/kg <==========

HYDROWIN Program (v2.00) Results:
==========
SMILES: O=C
CHEM: Formaldehyde
MOL FOR: C1 H2 O1
MOL WT: 30.03
---------- HYDROWIN v2.00 Results ----------

Currently, this program can NOT estimate a hydrolysis rate constant for
the type of chemical structure entered!!

ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens),
Specific Alkyl Halides & Phosphorus Esters can be estimated!!

When present, various hydrolyzable compound-types will be identified.
For more information, (Click OVERVIEW in Help or see the User's Guide)

***** CALCULATION NOT PERFORMED *****

BCFBAF Program (v3.01) Results:
==========
SMILES: O=C
CHEM: Formaldehyde
MOL FOR: C1 H2 O1
MOL WT: 30.03
---------- BCFBAF v3.01 ----------
Summary Results:
Log BCF (regression-based estimate): 0.50 (BCF = 3.16 L/kg wet-wt)
Biotransformation Half-Life (days) : 0.055 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): 0.02 (BAF = 1.06 L/kg wet-wt)

Log Kow (experimental): 0.35
Log Kow used by BCF estimates: 0.35 (user entered)

Equation Used to Make BCF estimate:
Log BCF = 0.50

Correction(s): Value
Correction Factors Not Used for Log Kow < 1

Estimated Log BCF = 0.500 (BCF = 3.162 L/kg wet-wt)

```
============================================================
Whole Body Primary Biotransformation Rate Estimate for Fish:
============================================================
------+-----+-----------------------------------------+---------+---------
TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
Frag |  1  |  Aldehyde   [-CHO]                      |  0.2465 |  0.2465
L Kow|  *  |  Log Kow =   0.35 (user-entered   )     |  0.3073 |  0.1076
MolWt|  *  |  Molecular Weight Parameter             |         | -0.0770
Const|  *  |  Equation Constant                      |         | -1.5371
============+=========================================+=========+======
===
RESULT   |       LOG Bio Half-Life (days)           |         | -1.2600
RESULT   |          Bio Half-Life (days)            |         | 0.05495
NOTE     |  Bio Half-Life Normalized to 10 g fish at 15 deg C   |
============+=========================================+=========+======
===
```

Biotransformation Rate Constant:
kM (Rate Constant): 12.61 /day (10 gram fish)
kM (Rate Constant): 7.093 /day (100 gram fish)
kM (Rate Constant): 3.989 /day (1 kg fish)
kM (Rate Constant): 2.243 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) = 0.024 (BCF = 1.056 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 0.024 (BAF = 1.056 L/kg wet-wt)
Estimated Log BCF (mid trophic)   = 0.024 (BCF = 1.058 L/kg wet-wt)
Estimated Log BAF (mid trophic)   = 0.024 (BAF = 1.058 L/kg wet-wt)
Estimated Log BCF (lower trophic) = 0.023 (BCF = 1.054 L/kg wet-wt)
Estimated Log BAF (lower trophic) = 0.023 (BAF = 1.054 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = 0.054 (BCF = 1.132 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 0.055 (BAF = 1.136 L/kg wet-wt)

Volatilization From Water
=========================
Chemical Name: Formaldehyde

Molecular Weight   : 30.03 g/mole
Water Solubility   : 5.5E+005 ppm
Vapor Pressure   : 3890 mm Hg
Henry's Law Constant: 3.37E-007 atm-m3/mole (entered by user)

```
RIVER           LAKE
---------       ---------
Water Depth     (meters):   1               1
```

Wind Velocity (m/sec): 5 0.5
Current Velocity (m/sec): 1 0.05

HALF-LIFE (hours) : 952.6 1.044E+004
HALF-LIFE (days) : 39.69 434.9
HALF-LIFE (years) : 0.1087 1.191

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
==========
(using 10000 hr Bio P,A,S)
PROPERTIES OF: Formaldehyde

Molecular weight (g/mol) 30.03
Aqueous solubility (mg/l) 550000
Vapour pressure (Pa) 518624
(atm) 5.11842
(mm Hg) 3890
Henry's law constant (Atm-m3/mol) 3.37E-007
Air-water partition coefficient 1.37823E-005
Octanol-water partition coefficient (Kow) 2.23872
Log Kow 0.35
Biomass to water partition coefficient 1.24774
Temperature [deg C] 25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
-Primary tank 0.03 24.89 10000.00
-Aeration tank 0.03 24.89 10000.00
-Settling tank 0.03 24.89 10000.00

STP Overall Chemical Mass Balance:
---
g/h mol/h percent

Influent 1.00E+001 3.3E-001 100.00

Primary sludge 2.55E-002 8.5E-004 0.25
Waste sludge 1.51E-001 5.0E-003 1.51
Primary volatilization 1.83E-004 6.1E-006 0.00
Settling volatilization 5.00E-004 1.7E-005 0.00
Aeration off gas 1.23E-003 4.1E-005 0.01

Primary biodegradation 1.76E-003 5.9E-005 0.02
Settling biodegradation 5.27E-004 1.8E-005 0.01
Aeration biodegradation 6.94E-003 2.3E-004 0.07

Final water effluent 9.81E+000 3.3E-001 98.13

Total removal 1.87E-001 6.2E-003 1.87

Total biodegradation 9.22E-003 3.1E-004 0.09

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
==========
(using Biowin/EPA draft method)
PROPERTIES OF: Formaldehyde

Molecular weight (g/mol) 30.03
Aqueous solubility (mg/l) 550000
Vapour pressure (Pa) 518624
(atm) 5.11842
(mm Hg) 3890
Henry's law constant (Atm-m3/mol) 3.37E-007
Air-water partition coefficient 1.37823E-005
Octanol-water partition coefficient (Kow) 2.23872
Log Kow 0.35
Biomass to water partition coefficient 1.24774
Temperature [deg C] 25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
-Primary tank 27.84 0.02 10.00
-Aeration tank 278.39 0.00 1.00
-Settling tank 278.39 0.00 1.00

STP Overall Chemical Mass Balance:
---
g/h mol/h percent

Influent 1.00E+001 3.3E-001 100.00

Primary sludge 2.17E-002 7.2E-004 0.22
Waste sludge 1.22E-002 4.1E-004 0.12
Primary volatilization 1.56E-004 5.2E-006 0.00
Settling volatilization 4.04E-005 1.3E-006 0.00
Aeration off gas 1.29E-004 4.3E-006 0.00

Primary biodegradation 1.50E+000 5.0E-002 14.96
Settling biodegradation 4.26E-001 1.4E-002 4.26
Aeration biodegradation 7.25E+000 2.4E-001 72.50

Final water effluent 7.93E-001 2.6E-002 7.93

Total removal 9.21E+000 3.1E-001 92.07
Total biodegradation 9.17E+000 3.1E-001 91.72

Level III Fugacity Model (Full-Output):
==========
Chem Name : Formaldehyde
Molecular Wt: 30.03

Henry's LC: 3.37e-007 atm-m3/mole (user-entered)
Vapor Press: 3.89e+003 mm Hg (user-entered)
Log Kow: 0.35 (user-entered)
Soil Koc: 1 (KOCWIN MCI method)

Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air 2.13	27.4	1000
Water 44.1	360	1000
Soil 53.6	720	1000
Sediment 0.0826	3.24e+003	0

Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air 2.03e-010	631	250	21	8.32
Water 2.9e-011	996	518	33.2	17.3
Soil 1.21e-009	605	0	20.2	0
Sediment 2.65e-011	0.207	0.0194	0.00691	0.000646

Persistence Time: 391 hr
Reaction Time: 525 hr
Advection Time: 1.53e+003 hr
Percent Reacted: 74.4
Percent Advected: 25.6

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 27.41
Water: 360
Soil: 720
Sediment: 3240
Biowin estimate: 3.155 (weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

....

B.2 EPISuite™ Results for Methylene Glycol

SMILES: C(O)O
CHEM: Methylene glycol
MOL FOR: C1 H4 O2
MOL WT: 48.04
---------- EPI SUMMARY (v4.11) ----------
Physical Property Inputs:
Log Kow (octanol-water): -0.79
Boiling Point (deg C): 131.60
Melting Point (deg C): -43.80
Vapor Pressure (mm Hg): 3.11
Water Solubility (mg/L): 1E+014
Henry LC (atm-m3/mole): 1.65E-007

KOWWIN Program (v1.68) Results:
==========
Log Kow(version 1.68 estimate): -0.79

SMILES: C(O)O
CHEM:
MOL FOR: C1 H4 O2
MOL WT: 48.04

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH2- [aliphatic carbon]	0.4911	0.4911
Frag	2	-OH [hydroxy, aliphatic attach]	-1.4086	-2.8172
Factor	1	Multi-alcohol correction	0.4064	0.4064
Factor	1	HO-C-OH (poly-alcohol carbon) correction	0.9000**	0.9000
Const		Equation Constant		0.2290
NOTE		An estimated coefficient (**) used		

Log Kow = -0.7907

MPBPVP (v1.43) Program Results:
==========
Experimental Database Structure Match: no data

SMILES: C(O)O
CHEM:
MOL FOR: C1 H4 O2
MOL WT: 48.04
---------- SUMMARY MPBVP v1.43 ----------
Boiling Point: 131.16 deg C (Adapted Stein and Brown Method)

Melting Point: -50.49 deg C (Adapted Joback Method)
Melting Point: -37.08 deg C (Gold and Ogle Method)
Mean Melt Pt : -43.78 deg C (Joback; Gold,Ogle Methods)
Selected MP: -43.78 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 131.60 deg C (user entered))
(MP not used for liquids)
VP: 3.32 mm Hg (Antoine Method)
: 443 Pa (Antoine Method)
VP: 2.75 mm Hg (Modified Grain Method)
: 367 Pa (Modified Grain Method)
VP: 11.9 mm Hg (Mackay Method)
: 1.59E+003 Pa (Mackay Method)
Selected VP: 3.04 mm Hg (Mean of Antoine & Grain methods)
: 405 Pa (Mean of Antoine & Grain methods)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH2-	24.22	24.22
Group	2	-OH (primary)	88.46	176.92
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		399.32
RESULT- corr		BOILING POINT in deg Kelvin		404.32
		BOILING POINT in deg C		131.16

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CH2-	11.27	11.27
Group	2	-OH (primary)	44.45	88.90
*		Equation Constant		122.50
RESULT		MELTING POINT in deg Kelvin		222.67
		MELTING POINT in deg C		-50.49

Water Sol from Kow (WSKOW v1.42) Results:
==========
Water Sol: 9.598e+005 mg/L
SMILES: C(O)O
CHEM:
MOL FOR: C1 H4 O2
MOL WT: 48.04

---------- WSKOW v1.42 Results ----------
Log Kow (estimated) : -0.79
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: -0.79 (user entered)

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction

Melting Pt (Tm) = -43.80 deg C (Use Tm = 25 for all liquids)

Correction(s): Value
---------- -----
No Applicable Correction Factors

Log Water Solubility (in moles/L) : 1.301
Water Solubility at 25 deg C (mg/L): 9.598e+005

WATERNT Program (v1.01) Results:
==========
Water Sol (v1.01 est): 1e+006 mg/L

SMILES: C(O)O
CHEM:
MOL FOR: C1 H4 O2
MOL WT: 48.04

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH2- [aliphatic carbon]	-0.5370	-0.5370
Frag	2	-OH [hydroxy, aliphatic attach]	1.6012	3.2025
Const		Equation Constant		0.2492
NOTE		Maximum Solubility (1,000,000 mg/L) Applied!		

Log Water Sol (moles/L) at 25 dec C = 1.3184
Water Solubility (mg/L) at 25 dec C = 1e+006

ECOSAR Program (v1.11) Results:
==========
ECOSAR Version 1.11 Results Page
SMILES: C(O)O
CHEM:
CAS Num:

ChemID1:
MOL FOR: C1 H4 O2
MOL WT: 48.04
Log Kow: -0.791 (EPISuite Kowwin v1.68 Estimate)
Log Kow: (User Entered)
Log Kow: (PhysProp DB exp value - for comparison only)
Melt Pt: -43.80 (deg C, User Entered for Wat Sol estimate)
Melt Pt: (deg C, PhysProp DB exp value for Wat Sol estimate)
Wat Sol: 9.613E+005 (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol: 1E+014 (mg/L, User Entered)
Wat Sol: (PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log Kow: -0.791 (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 1E+014 (mg/L, User Entered)

ECOSAR v1.11 Class-specific Estimations

Neutral Organics
Predicted

ECOSAR Class	Organism	Duration	End Pt	mg/L (ppm)
Neutral Organics	: Fish	96-hr	LC50	12663.330
Neutral Organics	: Daphnid	48-hr	LC50	5557.004
Neutral Organics	: Green Algae	96-hr	EC50	1426.405
Neutral Organics	: Fish	ChV		913.372
Neutral Organics	: Daphnid	ChV		264.544
Neutral Organics	: Green Algae	ChV		210.442
Neutral Organics	: Fish (SW)	96-hr	LC50	15678.052
Neutral Organics	: Mysid	96-hr	LC50	77164.227
Neutral Organics	: Fish (SW)	ChV		309.598
Neutral Organics	: Mysid (SW)	ChV		15250.326
Neutral Organics	: Earthworm	14-day	LC50	162.636

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs

presented below, then no effects at saturation are expected for those endpoints.

Neutral Organics:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
Maximum LogKow: 6.0 (Earthworm LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)

HENRYWIN (v3.20) Program Results:
==========
Bond Est : 9.85E-008 atm-m3/mole (9.98E-003 Pa-m3/mole)
Group Est: 1.07E-008 atm-m3/mole (1.08E-003 Pa-m3/mole)

SMILES: C(O)O
CHEM:
MOL FOR: C1 H4 O2
MOL WT: 48.04
---------- HENRYWIN v3.20 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	2 Hydrogen to Carbon (aliphatic) Bonds		-0.2394
HYDROGEN	2 Hydrogen to Oxygen Bonds		6.4635
FRAGMENT	2 C-O		2.1709
FACTOR	1 Additional aliphatic alcohol -OH(s)		-3.0000
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	5.395

HENRYs LAW CONSTANT at 25 deg C = 9.85E-008 atm-m3/mole
= 4.03E-006 unitless
= 9.98E-003 Pa-m3/mole

GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
1 CH2 (O)(O)		-2.54
2 O-H (C)		8.90
RESULT	GROUP ESTIMATION METHOD for LOG GAMMA VALUE	TOTAL	6.36

HENRYs LAW CONSTANT at 25 deg C = 1.07E-008 atm-m3/mole
= 4.37E-007 unitless
= 1.08E-003 Pa-m3/mole

For Henry LC Comparison Purposes:

Exper Database: none available
User-Entered Henry LC: 1.650E-007 atm-m3/mole (1.672E-002 Pa-m3/mole)
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 1.966E-015 atm-m3/mole (1.992E-010 Pa-m3/mole)
VP: 3.11 mm Hg (source: User-Entered)
WS: 1E+014 mg/L (source: User-Entered)

Log Octanol-Air (KOAWIN v1.10) Results:
==========
Log Koa: 4.381

SMILES: C(O)O
CHEM:
MOL FOR: C1 H4 O2
MOL WT: 48.04
---------- KOAWIN v1.10 Results ----------
Log Koa (octanol/air) estimate: 4.381
Koa (octanol/air) estimate: 2.404e+004
Using:
Log Kow: -0.79 (user entered)
HenryLC: 1.65e-007 atm-m3/mole (user entered)
Log Kaw: -5.171 (air/water part.coef.)

LogKow: ---- (exp database)
LogKow: -0.79 (KowWin estimate)
Henry LC: --- atm-m3/mole(exp database)
Henry LC: 9.85e-008 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate: 4.605 (from KowWin/HenryWin)

BIOWIN (v4.10) Program Results:
==========
SMILES: C(O)O
CHEM:
MOL FOR: C1 H4 O2
MOL WT: 48.04
---------- BIOWIN v4.10 Results ----------
Biowin1 (Linear Model Prediction): Biodegrades Fast
Biowin2 (Non-Linear Model Prediction): Biodegrades Fast
Biowin3 (Ultimate Biodegradation Timeframe): Days-Weeks
Biowin4 (Primary Biodegradation Timeframe): Days
Biowin5 (MITI Linear Model Prediction): Biodegrades Fast
Biowin6 (MITI Non-Linear Model Prediction): Biodegrades Fast
Biowin7 (Anaerobic Model Prediction): Biodegrades Fast
Ready Biodegradability Prediction: YES

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aliphatic alcohol [-OH]	0.1587	0.3175
MolWt	*	Molecular Weight Parameter		-0.0229
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		1.0421

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aliphatic alcohol [-OH]	1.1178	2.2356
MolWt	*	Molecular Weight Parameter		-0.6822
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.9897

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aliphatic alcohol [-OH]	0.1600	0.3199
MolWt	*	Molecular Weight Parameter		-0.1062
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		3.4129

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aliphatic alcohol [-OH]	0.1294	0.2589
MolWt	*	Molecular Weight Parameter		-0.0693
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		4.0373

```
============+==========================================+=========+======
===

Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
(Primary & Ultimate)    2.00 -> months    1.00 -> longer

------+-----+------------------------------------------+---------+---------
TYPE | NUM |      Biowin5 FRAGMENT DESCRIPTION        | COEFF  |  VALUE
------+-----+------------------------------------------+---------+---------
Frag |  2  |  Aliphatic alcohol  [-OH]                | 0.1611 |  0.3223
Frag |  1  |  -CH2-  [linear]                         | 0.0494 |  0.0494
MolWt|  *  |  Molecular Weight Parameter              |        | -0.1429
Const|  *  |  Equation Constant                       |        |  0.7121
============+==========================================+=========+======
===
RESULT   |  Biowin5 (MITI Linear Biodeg Probability)  |        |  0.9409
============+==========================================+=========+======
===

------+-----+------------------------------------------+---------+---------
TYPE | NUM |      Biowin6 FRAGMENT DESCRIPTION        | COEFF  |  VALUE
------+-----+------------------------------------------+---------+---------
Frag |  2  |  Aliphatic alcohol  [-OH]                |  1.0041 |  2.0083
Frag |  1  |  -CH2-  [linear]                         | 0.4295 |  0.4295
MolWt|  *  |  Molecular Weight Parameter              |        | -1.3869
============+==========================================+=========+======
===
RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|        |  0.9728
============+==========================================+=========+======
===

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable


------+-----+------------------------------------------+---------+---------
TYPE | NUM |      Biowin7 FRAGMENT DESCRIPTION        | COEFF  |  VALUE
------+-----+------------------------------------------+---------+---------
Frag |  2  |  Aliphatic alcohol  [-OH]                | 0.1328 |  0.2655
Frag |  1  |  -CH2-  [linear]                         | 0.0260 |  0.0260
Const|  *  |  Equation Constant                       |        |  0.8361
============+==========================================+=========+======
===
RESULT   |   Biowin7 (Anaerobic Linear Biodeg Prob)   |        |  1.1276
============+==========================================+=========+======
===
A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast
```

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

BioHCwin (v1.01) Program Results:
==========
SMILES: C(O)O
CHEM:
MOL FOR: C1 H4 O2
MOL WT: 48.04
---------- BioHCwin v1.01 Results ----------

NO Estimate Possible ... Structure NOT a Hydrocarbon
(Contains atoms other than C, H or S (-S-))

AEROWIN Program (v1.00) Results:
==========
Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 415 Pa (3.11 mm Hg)
Log Koa (Koawin est): 4.381
Kp (particle/gas partition coef. (m3/ug)):
Mackay model: 7.23E-009
Octanol/air (Koa) model: 5.9E-009
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model: 2.61E-007
Mackay model: 5.79E-007
Octanol/air (Koa) model: 4.72E-007

AOP Program (v1.92) Results:
==========
SMILES: C(O)O
CHEM:
MOL FOR: C1 H4 O2
MOL WT: 48.04
---------- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) --------

Hydrogen Abstraction = 11.4415 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.2800 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 11.7215 E-12 cm3/molecule-sec
HALF-LIFE = 0.913 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 10.950 Hrs
---------- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches
Fraction sorbed to airborne particulates (phi):
4.2E-007 (Junge-Pankow, Mackay avg)
4.72E-007 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

KOCWIN Program (v2.00) Results:
==========
SMILES: C(O)O
CHEM:
MOL FOR: C1 H4 O2
MOL WT: 48.04
---------- KOCWIN v2.00 Results ----------
Koc Estimate from MCI:

First Order Molecular Connectivity Index ..... : 1.414
Non-Corrected Log Koc (0.5213 MCI + 0.60) ..... : 1.3370
Fragment Correction(s):
2 Aliphatic Alcohol (-C-OH) ..... : -2.6358
Corrected Log Koc ..... : -1.2988
Over Correction Adjustment to Lower Limit Log Koc ... : 0.0000

Estimated Koc: 1 L/kg <==========

Koc Estimate from Log Kow:

Log Kow (User entered) ..... : -0.79
Non-Corrected Log Koc (0.55313 logKow + 0.9251) .... : 0.4881
Fragment Correction(s):
2 Aliphatic Alcohol (-C-OH) ..... : -0.8229
Corrected Log Koc ..... : -0.3348

Estimated Koc: 0.4626 L/kg   <==========

HYDROWIN Program (v2.00) Results:
==========
SMILES: C(O)O
CHEM:
MOL FOR: C1 H4 O2
MOL WT: 48.04
---------- HYDROWIN v2.00 Results ----------
Currently, this program can NOT estimate a hydrolysis rate constant for
the type of chemical structure entered!!

ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens),
Specific Alkyl Halides & Phosphorus Esters can be estimated!!

When present, various hydrolyzable compound-types will be identified.
For more information, (Click OVERVIEW in Help or see the User's Guide)

*****   CALCULATION NOT PERFORMED   *****

BCFBAF Program (v3.01) Results:
==========
SMILES: C(O)O
CHEM:
MOL FOR: C1 H4 O2
MOL WT: 48.04
---------- BCFBAF v3.01 ----------
Summary Results:
Log BCF (regression-based estimate): 0.50 (BCF = 3.16 L/kg wet-wt)
Biotransformation Half-Life (days): 0.00995 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): -0.05 (BAF = 0.898 L/kg wet-wt)

Log Kow (experimental): not available from database
Log Kow used by BCF estimates: -0.79 (user entered)

Equation Used to Make BCF estimate:
Log BCF = 0.50

Correction(s):   Value
Correction Factors Not Used for Log Kow < 1

Estimated Log BCF = 0.500 (BCF = 3.162 L/kg wet-wt)

==========
Whole Body Primary Biotransformation Rate Estimate for Fish:

```
============================================================
------+-----+-----------------------------------------+---------+---------
TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
Frag |  2  |  Aliphatic alcohol  [-OH]                | -0.0616 | -0.1231
Frag |  1  |  -CH2-  [linear]                         |  0.0242 |  0.0242
L Kow|  *  |  Log Kow =  -0.79 (user-entered  )       |  0.3073 | -0.2428
MolWt|  *  |  Molecular Weight Parameter              |         | -0.1232
Const|  *  |  Equation Constant                       |         | -1.5371
============+=============================================+=========+======
===
RESULT   |       LOG Bio Half-Life (days)          |         | -2.0020
RESULT   |          Bio Half-Life (days)           |         |0.009954
NOTE     |  Bio Half-Life Normalized to 10 g fish at 15 deg C   |
============+=============================================+=========+======
===
```

Biotransformation Rate Constant:
kM (Rate Constant): 69.63 /day (10 gram fish)
kM (Rate Constant): 39.16 /day (100 gram fish)
kM (Rate Constant): 22.02 /day (1 kg fish)
kM (Rate Constant): 12.38 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) = -0.047 (BCF = 0.8979 L/kg wet-wt)
Estimated Log BAF (upper trophic) = -0.047 (BAF = 0.8979 L/kg wet-wt)
Estimated Log BCF (mid trophic)   = -0.028 (BCF = 0.9366 L/kg wet-wt)
Estimated Log BAF (mid trophic)   = -0.028 (BAF = 0.9366 L/kg wet-wt)
Estimated Log BCF (lower trophic) = -0.024 (BCF = 0.9452 L/kg wet-wt)
Estimated Log BAF (lower trophic) = -0.024 (BAF = 0.9452 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = -0.041 (BCF = 0.9103 L/kg wet-wt)
Estimated Log BAF (upper trophic) = -0.041 (BAF = 0.9106 L/kg wet-wt)

Volatilization From Water
=========================

Chemical Name:

Molecular Weight: 48.04 g/mole
Water Solubility: 1E+014 ppm
Vapor Pressure: 3.11 mm Hg
Henry's Law Constant: 1.65E-007 atm-m3/mole (entered by user)

	RIVER	LAKE
Water Depth (meters):	1	1

Wind Velocity (m/sec): 5 0.5
Current Velocity (m/sec): 1 0.05

HALF-LIFE (hours): 2460 2.69E+004
HALF-LIFE (days): 102.5 1121
HALF-LIFE (years): 0.2806 3.068

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
==========
(using Biowin/EPA draft method)
PROPERTIES OF:

Molecular weight (g/mol) 48.04
Aqueous solubility (mg/l) 1E+014
Vapour pressure (Pa) 414.633
(atm) 0.00409211
(mm Hg) 3.11
Henry 's law constant (Atm-m3/mol) 1.65E-007
Air-water partition coefficient 6.74801E-006
Octanol-water partition coefficient (Kow) 0.162181
Log Kow -0.79
Biomass to water partition coefficient 0.832436
Temperature [deg C] 25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
-Primary tank 41.69 0.02 10.00
-Aeration tank 416.94 0.00 1.00
-Settling tank 416.94 0.00 1.00

STP Overall Chemical Mass Balance:
---
g/h mol/h percent

Influent	1.00E+001	2.1E-001	100.00
Primary sludge	2.13E-002	4.4E-004	0.21
Waste sludge	1.22E-002	2.5E-004	0.12
Primary volatilization	7.65E-005	1.6E-006	0.00
Settling volatilization	1.98E-005	4.1E-007	0.00
Aeration off gas	6.32E-005	1.3E-006	0.00
Primary biodegradation	1.50E+000	3.1E-002	14.95
Settling biodegradation	4.26E-001	8.9E-003	4.26
Aeration biodegradation	7.25E+000	1.5E-001	72.51
Final water effluent	7.94E-001	1.7E-002	7.94
Total removal	9.21E+000	1.9E-001	92.06
Total biodegradation	9.17E+000	1.9E-001	91.72

Level III Fugacity Model (Full-Output):
==========

Chem Name:
Molecular Wt: 48.04
Henry's LC: 1.65e-007 atm-m3/mole (user-entered)
Vapor Press: 3.11 mm Hg (user-entered)
Log Kow: -0.79 (user-entered)
Soil Koc: 1 (KOCWIN MCI method)

Mass Amount	Half-Life (percent)	(hr)	Emissions (kg/hr)
Air	2.18	21.9	1000
Water	39	208	1000
Soil	58.8	416	1000
Sediment	0.0689	1.87e+003	0

Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)	
Air	9.3e-011	578	183	19.3	6.09
Water	5.62e-012	1.09e+003	327	36.3	10.9
Soil	2.91e-010	822	0	27.4	0
Sediment	4.85e-012	0.214	0.0116	0.00713	0.000386

Persistence Time: 280 hr
Reaction Time: 337 hr
Advection Time: 1.65e+003 hr
Percent Reacted: 83
Percent Advected: 17

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 21.9
Water: 208.1
Soil: 416.2
Sediment: 1873
Biowin estimate: 3.413 (days-weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004