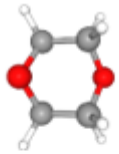
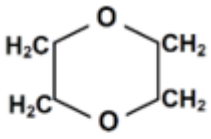
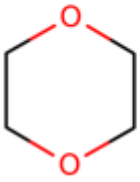
Appendix B: 1,4-Dioxane Identifiers and the Physical and Chemical Properties of 1,4-Dioxane

Table 1. 1,4-Dioxane Identifiers

Chemical Name	1,4-dioxane
CAS Registry No.	123-91-1
NIOSH RTECS No.	JG8225000
FDA UNII	J8A3S10O7S
DOT ID and Response Guide No.	1165; Guide 127
USEPA Hazardous Waste ID No.	U108
PubChem CID	31275
Beilstein Reference No.	102551
Other Names	Para-Dioxane, p-Dioxane, 1,4-Diethylene dioxide, 1,4-Dioxacyclohexane, Di(ethylene oxide), Diethylene dioxide, Diethylene ether, Diokan, Dioksan (Polish), Diossano-1,4 (Italian), Dioxaan-1,4 (Dutch), Dioxan, Dioxan-1,4 (German), Dioxane, Dioxane-1,4, Dioxanne (French), Dioxyethylene ether, Glycol ethylene ether, NCI-C03689, p-Dioxan (Czech), RCRA waste number U108, Tetrahydro-1,4-dioxin, Tetrahydro-p-dioxin (NIH 2020)
Chemical Formula	$C_4H_8O_2$
Chemical Structure	  
SMILES	O(CCOC1)C1
Major Chemical Class	Heterocyclic organic compound, classified as an ether

Physical State, Color, Odor at 15°C	Colorless liquid that can also be a solid below 53°F (11.67°C). Very flammable, volatile liquid with a faint, pleasant, ether-like odor. Vapor harmful. (O'Neil et al. 2001; USCG 1999; ATSDR 2012; ECB 2002; Montgomery 2007)
Grades	ACS Reagent (≥99%), anhydrous (99.8%), HPLC (≥99.9%), technical (≥95%) (Sigma Aldrich Co. 2019)
Common Impurities	Bis(2-Chloroethyl) ether (<0.1%); Water (<0.1%); 2-Methyl-1, 3-dioxane (<0.1%); 2-Ethyl-1, 3-dioxane (≤0.001%); Hydrogen peroxide (≤0.001%); Lead (≤0.25 ppm); Iron (0.25 ppm) (ECB 2002)
Preparation	Commercially prepared by heating diethylene glycol in the presence of sulfuric acid (H_2SO_4) (Surprenant 2012; American Chemical Society 2019)
Molecular Weight	88.106 g/mole (Riddick, Bunger, and Sakano 1986; Mackay et al. 2006; Daubert et al. 1989)
Other	Hydrogen bond acceptor count = 2; Covalently bonded unit count = 1; Polar surface area = 18.5Å^2. May form explosive peroxides (especially when anhydrous) (NCBI 2020).

Table 2. Physical and Chemical Properties of 1,4-Dioxane

Property	**Units**	**Value**	**Source**
Acid dissociation constant pK_a	No units	–2.92	(Mohr et al. 2010)
Autoignition temperature	°C	180	(USCG 1999; Daubert et al. 1989)
Azeotropic data for 1,4-dioxane–water mixture	At boiling point = 87.82°C	82% w dioxane 18% w water	(Horsley 1947)
Boiling point	°C	101.5	(Lide and Haynes 2009)
Critical pressure	MPa	5.21 (51.4 atm)	(Riddick, Bunger, and Sakano 1986; USCG 1999; Daubert et al. 1989)
Critical temperature	°C	314	(Daubert et al. 1989; Riddick, Bunger, and Sakano 1986; USCG 1999)
Diffusivity in air	(x 10^{-2} cm^2/sec at 25°C)	8.7	(USEPA 2001)[MG1]
Diffusivity in water	(x 10^{-5} cm^2/sec at 25°C) value strongly dependent on composition of aqueous phase	0.32 to 2.38	(Leaist et al. 2000; Montgomery 2007)
Ebullioscopic constant	°C kg/mol	3.01	(Lide and Haynes 2009)
Electric dipole moment	debyes	0.4	(Mohr et al. 2010)
Flammability limits in air	Vol % 1 atm, 25°C	2 to 22%	(Coronado et al. 2012; Daubert et al. 1989; Surprenant 2012)

Flash point	°C (closed cup)	12.2	(Daubert et al. 1989; USCG 1999)
	°C (open cup)	23.3	(USCG 1999)
Freezing point	°C	11.8	(Riddick, Bunger, and Sakano 1986; USCG 1999)
Gas phase (atmospheric) OH radical rate constan	(x 10^{12} cm^3 $molecule^{-1}$-sec^{-1} at 25°C)	10.91 +/- 0.5	(Atkinson 1989)
Heat capacity	J mol^{-1} K^{-1} at 25 C	150.65	(Grolier, Inglese, and Wilhelm 1984)
Heat of fusion	kJ/mol	12.46	(Riddick, Bunger, and Sakano 1986; Mohr et al. 2010; O'Neil et al. 2001)
Heat of vaporization	kJ/mol	38.60 at 25°C	(Lide and Haynes 2009)
		34.16 at 101.5°C	(Lide and Haynes 2009)
Henry's law volatility constant	Pa m^3/mol at 25°C	0.486 (4.80 × 10^{-6} atm m^3/mol)	(USEPA and SRC 2019; USEPA 2018[MG2] ; Park et al. 1987; NCBI 2020; ATSDR 2012)
Hildebrand solubility parameter	x 10^4 $(J/m^3)^{1/2}$	2.0163	(Daubert et al. 1989)
Ionization potential	eV	9.19 +/- 0.01	(Fraser-Monteiro et al. 1982)
Liquid density	g/cm^3 at 20°C	1.0337	(Lide and Haynes 2009)
	g/cm^3 at 25°C	1.028	(Abraham et al. 1971; Hovorka et al. 1936; Reyes et al. 2003; Riddick, Bunger, and Sakano 1986)
Liquid molar volume	cm^3/mol	85.7	(Daubert et al. 1989)
Liquid surface tension	mN/m at 25°C	32.75	(Rafati et al. 2009; Jasper 1972; Lide and Haynes 2009)
Liquid thermal conductivity	W/m K at 25°C	0.159	(Lide and Haynes 2009)
Liquid viscosity	mPa s at 25°C	1.177	(Lide and Haynes 2009)
n-octanol/air partition coefficient, log K_{OA}	No units at 25°C	3.17	(Abraham et al. 2001; Mackay et al. 2006; USEPA et al. 2019)

n-octanol/water partition coefficient (Log K_{ow}) Odor threshold	No units Weight/volume (w/v)	–0.27 at 20°C	(Hansch and Leo 1979; Barone, Rowe, and Quigley 1992)
		–0.42 at 20°C	(Collander 1951; Chou and Jurs 1979)
		230 ppm in water	(Amoore and Hautala 1983)
	Volume/volume (v/v)	24 ppm in air	(ATSDR 2012)
Organic carbon-water partition coefficient (Log K_{oc})	No units	0.42	(USEPA and SRC 2019)
		1.23	(HSDB 2019; Schüürmann, Ebert, and Kühne 2006; Huuskonen 2003)
		1.46	(Barone, Rowe, and Quigley 1992; HSDB 2019)
Refractive index	No units (at 20°C)	1.4224	(Lide and Haynes 2009)
Relative evaporation rate	Relative to butyl acetate = 1	2.42	(Mohr et al. 2010)
	Relative to Diethyl Ether = 1	7.3	(NICNAS 1998)
Relative permittivity or dielectric constant	No units at 25 °C	2.209	(Papanastasiou, Papoutsis, and Kokkinidis 1987; Maryott and Smith 1951)
Standard heat of entropy	J mol^{-1} K^{-1}	270.2	(Lide and Haynes 2009)
Standard heat of formation—liquid	kJ/mol	–355.13 +/- 0.86	(Byström and Månsson 1982)
Trouton constant	J $mol^{-1}K^{-1}$	21.90	(O'Neil et al. 2001)
Ultraviolet light absorption maximum	nm	180	(Mohr et al. 2010)
Vapor density (relative to air = 1)	No units at 25°C	3.06	(Mohr et al. 2010)
Vapor pressure	kPa at 20° C	3.90 (29 mm Hg)	(NIOSH 1994; Crenshaw et al. 1938)
	kPa at 25°C	5.08 (38.1 mm Hg)	(Banerjee, Howard, and Lande 1990; Daubert et al. 1989; USEPA et al. 2019)
Water solubility	g/L at 25°C	1,000	(USEPA and SRC 2019; Riddick, Bunger, and Sakano 1986)

Other solubility data	No units	Soluble in acetone, alcohol, benzene, and ether. Miscible with most organic solvents, including 2-methylpropanol, toluene, cyclohexanone, and cyclopentanone.	(Weast and Astle 1986; Huntress and Mulliken 1941)

Notes:

Most properties have been obtained from commonly used handbooks, such as the *CRC Handbook of Chemistry and Physics* (Lide and Haynes 2009), *The Merck Index* (O'Neil et al. 2001), *Physical and Thermodynamic Properties of Pure Chemicals* (Daubert et al. 1989), and others. Other properties, such as aqueous solubility, vapor pressure, octanol-water partition coefficient, and Henry's law constant, have been obtained from scientific journals or other environmental handbooks. Other properties were also obtained from peer-reviewed data sets, such as PubChem (NCBI 2020), the USEPA chemistry dashboard (USEPA 2019a), USEPA Superfund Chemical specific screening data sets (USEPA 2019b), and others.

The emphasis in this table is on experimentally determined values rather than estimated values. Calculated or correlated values are viewed as being less reliable. The most reliable sources of data are the original citations of valuable experimental data in the reviewed scientific literature.

Properties vary depending on many variables. The aim of these tables has been to gather experimental data with a list of citations to interpret them and select a "best" or "most likely" value.

Scientific literature values for 1,4-dioxane's half-life were not reported. The half-life in the environment depends not only on the intrinsic properties of 1,4-dioxane but also on the nature of the environmental compartments. Factors such as sunlight intensity, hydroxyl radical concentration, and the nature of the microbial community, as well as the temperature, affect 1,4-dioxane's half-life. Literature values often do not take these factors into consideration, so it is misleading to document a single reliable half-life.