United States
Environmental Protection Agency

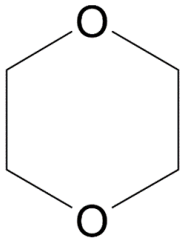
Office of Chemical Safety and
Pollution Prevention

Final Risk Evaluation for 1,4-Dioxane

Systematic Review Supplemental File:

Data Quality Evaluation of Environmental Fate and Transport Studies

CASRN: 123-91-1



December 2020

This document is a compilation of tables for the data extraction and evaluation for 1,4-Dioxane. Each table shows the data point or set or information element that was extracted and evaluated from a data source in accordance with Appendix D of the *Application of Systematic Review in TSCA Risk Evaluations*. If the source contains more than one data set or information element, the review provides an overall confidence score for each data set or information element that is found in the source. Therefore, it is possible that a source may have more than one overall quality/confidence score.

Table of Contents

Study Reference:	Kelley, S. L., Aitchison, E. W., Deshpande, M., Schnoor, J. L., Alvarez, P. J. J Biodegradation of 1,4-dioxane in planted and unplanted soil: Effect of bioaugmentation with Amycolata sp CB1190. Water Research. 2001. 35:3791-3800. HERO ID: 1462050					
Domain	**Metric**	**Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]**	**Comments**	**Metric Score**	**Metric Weighting Factor**	**Weighted Score**
Test Substance	1. Test substance identity	High	The test substance was identified by chemical name.	1	2	2
	2. Test substance purity	Medium	The source and purity of 1,4-dioxane were not reported under materials and methods; a brief description (p. 3797) of the tracer material was reported.	2	1	2
Test Design	3. Study Controls	Medium	Reference substance was not reported but some experimental controls were run with the test material.	2	2	4
	4. Test Substance stability	Medium	Details regarding this metric were not reported but this does not limit the interpretation of the results.	2	1	2
Test Conditions	5. Test Method Suitability	High	The test method was suitable for the test substance.	1	1	1
	6. Testing Conditions	Medium	Some testing conditions (soil details) were not provided; however, the omissions were not likely to have had a substantial impact on the study results.	2	2	4
	7. Testing Consistency	High	No inconsistencies were reported or identified.	1	1	1
	8. System Type and Design	High	System design was reported and appropriate.	1	1	1
Test Organisms	9. Test Organism Degradation	High	Pure culture test organism described.	1	2	2
	10. Test Organism Partitioning	Not rated (NR)	The metric is not applicable to this study type.	NR	NR	NR
Outcome Assessment	11. Outcome Assessment	Medium	The experiment with hybrid poplar trees	2	1	2

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Domain	**Metric**	**Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]**	**Comments**	**Metric Score**	**Metric Weighting Factor**	**Weighted Score**
	Methodology		evaluated dioxane removal by evapotranspiration and biodegradation and may not be relevant to typical environmental conditions.			
	12. Sampling Methods	Medium	The experiment with hybrid poplar trees evaluated dioxane removal by evapotranspiration and biodegradation and may not be relevant to typical environmental conditions.	2	1	2
Confounding/ Variable Control	13. Confounding Variables	Low	49-67% total recovery was reported; the authors indicated that the remaining 51-33% may have leaked from the system.	3	1	3
	14. Outcomes Unrelated to Exposure	Not rated	The metric is not applicable to this study type.	NR	NR	NR
Data Presentation and Analysis	15. Data Reporting	Medium	Some information was not reported (i.e., mass balance); however, these omissions were not likely to have had a substantial impact on the study results.	2	2	4
	16. Statistical Methods and Kinetic Calculations	Not rated	The metric is not applicable to this study type.	NR	NR	NR
Other	17. Verification or Plausibility of Results	Not rated	The metric is not applicable to this study type.	NR	NR	NR
	18. QSAR Models	Not rated	The metric is not applicable to this study type.	NR	NR	NR
			Sum of scores:	22	18	30

Study Reference:	Kelley, S. L., Aitchison, E. W., Deshpande, M., Schnoor, J. L., Alvarez, P. J. J Biodegradation of 1,4-dioxane in planted and unplanted soil: Effect of bioaugmentation with Amycolata sp CB1190. Water Research. 2001. 35:3791-3800. HERO ID: 1462050					
Domain	**Metric**	**Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]**	**Comments**	**Metric Score**	**Metric Weighting Factor**	**Weighted Score**
High	Medium	Low	**Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:**	1.67	**Overall Score (Rounded):**	1.7
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			**Overall Quality Level:**	Medium

Study Reference:	Boethling, R. S. and D. Mackay (2000). Handbook of property estimation methods for chemicals: Environmental and health sciences. Boca Raton, FL, Lewis. HERO ID: 196353					
Domain	**Metric**	**Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]**	**Comments**	**Metric Score**	**Metric Weighting Factor**	**Weighted Score**
Test Substance	1. Test substance identity	High	The test substance was identified by chemical name.	1	2	2
	2. Test substance purity	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Test Design	3. Study Controls	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	4. Test Substance stability	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Test Conditions	5. Test Method Suitability	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	6. Testing Conditions	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	7. Testing Consistency	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	8. System Type and Design	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Test Organisms	9. Test Organism Degradation	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	10. Test Organism Partitioning	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Outcome Assessment	11. Outcome Assessment Methodology	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	12. Sampling Methods	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Confounding/ Variable Control	13. Confounding Variables	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	14. Outcomes Unrelated to Exposure	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Data Presentation and Analysis	15. Data Reporting	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	16. Statistical Methods and Kinetic Calculations	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR

Study Reference:	Boethling, R. S. and D. Mackay (2000). Handbook of property estimation methods for chemicals: Environmental and health sciences. Boca Raton, FL, Lewis. HERO ID: 196353					
Domain	**Metric**	**Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]**	**Comments**	**Metric Score**	**Metric Weighting Factor**	**Weighted Score**
Other	17. Verification or Plausibility of Results	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	18. QSAR Models	High	Discusses mechanisms and QSAR models for hydrolysis such as HYDROWIN 1.67 which has a defined, unambiguous endpoint and model performance is known.	1	1	1
			Sum of scores:	2	3	3
High	Medium	Low	**Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:**	1	**Overall Score (Rounded):**	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			**Overall Quality Level:**	High

Study Reference:	U.S, EPA. 2012. Estimation Programs Interface Suite™ for Microsoft® Windows, version 4.11. HERO ID: 2347246					
Domain	**Metric**	**Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]**	**Comments**	**Metric Score**	**Metric Weighting Factor**	**Weighted Score**
Test Substance	1. Test substance identity	High	The test substance was identified by chemical name.	1	2	2
	2. Test substance purity	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Test Design	3. Study Controls	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	4. Test Substance stability	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Test Conditions	5. Test Method Suitability	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	6. Testing Conditions	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	7. Testing Consistency	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	8. System Type and Design	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Test Organisms	9. Test Organism Degradation	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	10. Test Organism Partitioning	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Outcome Assessment	11. Outcome Assessment Methodology	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	12. Sampling Methods	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Confounding/ Variable Control	13. Confounding Variables	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	14. Outcomes Unrelated to Exposure	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Data Presentation and Analysis	15. Data Reporting	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	16. Statistical Methods and Kinetic	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR

Study Reference:	U.S, EPA. 2012. Estimation Programs Interface Suite™ for Microsoft® Windows, version 4.11. HERO ID: 2347246					
Domain	**Metric**	**Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]**	**Comments**	**Metric Score**	**Metric Weighting Factor**	**Weighted Score**
	Calculations					
Other	17. Verification or Plausibility of Results	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	18. QSAR Models	High	The models in EPI Suite™ have defined endpoints. Chemical domain and performance statistics for each model are known, and unambiguous algorithms are available in the EPI Suite™ documentation and/or cited references to establish their scientific validity. Many EPI SuiteTM models have correlation coefficients >0.7, cross-validated correlation coefficients >0.5, and standard error values <0.3; however, correlation coefficients (r2, q2) for the regressions of some environmental fate models (i.e. BIOWIN) are lower, as expected, compared to regressions which have specific experimental values such as water solubility or log Kow (octanol-water partition coefficient).	1	1	1
			Sum of scores:	2	3	3

Study Reference:	U.S, EPA. 2012. Estimation Programs Interface Suite™ for Microsoft® Windows, version 4.11. HERO ID: 2347246					
Domain	**Metric**	**Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]**	**Comments**	**Metric Score**	**Metric Weighting Factor**	**Weighted Score**
High	Medium	Low	**Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:**	1	**Overall Score (Rounded):**	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			**Overall Quality Level:**	High

Study Reference:	Lyman, W., W. Reehl, and D. Ronsenblatt. 1982. Handbook of Chemical Property Estimation Methods (Ch 8, P 8-4). HERO ID: 4795691					
Domain	**Metric**	**Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]**	**Comments**	**Metric Score**	**Metric Weighting Factor**	**Weighted Score**
Test Substance	1. Test substance identity	High	The test substance was identified by chemical name.	1	2	2
	2. Test substance purity	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Test Design	3. Study Controls	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	4. Test Substance stability	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Test Conditions	5. Test Method Suitability	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	6. Testing Conditions	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	7. Testing Consistency	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	8. System Type and Design	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Test Organisms	9. Test Organism Degradation	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	10. Test Organism Partitioning	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Outcome Assessment	11. Outcome Assessment Methodology	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	12. Sampling Methods	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Confounding/ Variable Control	13. Confounding Variables	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	14. Outcomes Unrelated to Exposure	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
Data Presentation and Analysis	15. Data Reporting	High	This metric met the criteria for high confidence as expected for this type of study.	1	2	2
	16. Statistical	Not rated	The metric is not	NR	NR	NR

Study Reference:	Lyman, W., W. Reehl, and D. Ronsenblatt. 1982. Handbook of Chemical Property Estimation Methods (Ch 8, P 8-4). HERO ID: 4795691					
Domain	**Metric**	**Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]**	**Comments**	**Metric Score**	**Metric Weighting Factor**	**Weighted Score**
	Methods and Kinetic Calculations		applicable to this study type (SAR).			
Other	17. Verification or Plausibility of Results	Not rated	The metric is not applicable to this study type (SAR).	NR	NR	NR
	18. QSAR Models	High	The study data were based on a SAR for a compound with a known chemical structure.	1	1	1
			Sum of scores:	3	5	5
High	Medium	Low	**Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:**	1	**Overall Score (Rounded):**	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			**Overall Quality Level:**	High