United States
Environmental Protection Agency

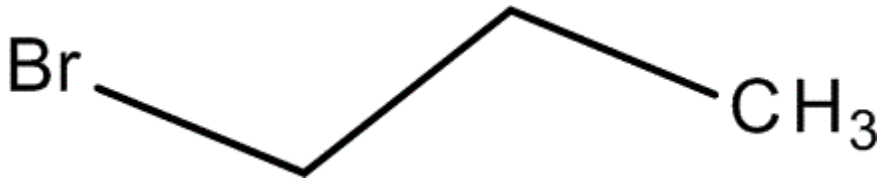
Office of Chemical Safety and
Pollution Prevention

Final Risk Evaluation for 1-Bromopropane (*n*-Propyl Bromide)

Systematic Review Supplemental File:

Data Quality Evaluation of Environmental Fate and Transport Studies

CASRN: 106-94-5



August 2020

Table of Contents

Study Reference:	Belkin, S. (1992). Biodegradation of Haloalkanes. In International Workshop on The Use of Microorganisms to Combat Pollution, Israel, May (pp. 10-18). (ISSN 0923-9820). HERO ID: 1737896					
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 common name, 1-bromopropane.	1	2	2
	2. Test Substance Purity	Not rated	The metric is not applicable to this review article.	NR	NR	NR
Test Design	3. Study Controls	Not rated	The metric is not applicable to this review article.	NR	NR	NR
	4. Test Substance Stability	Not rated	The metric is not applicable to this review article.	NR	NR	NR
Test Conditions	5. Test Method Suitability	Not rated	The metric is not applicable to this review article.	NR	NR	NR
	6. Testing Conditions	Not rated	The metric is not applicable to this review article.	NR	NR	NR
	7. Testing Consistency	Not rated	The metric is not applicable to this review article.	NR	NR	NR
	8. System Type and Design	Not rated	The metric is not applicable to this review article.	NR	NR	NR
Test Organisms	9. Test Organism Degradation	Medium	The test species were reported. The pure culture was not routinely used for environmentally relevant biodegradation studies.	2	2	4

	10. Test Organism Partitioning	Not rated	The metric is not applicable to this review article.	NR	NR	NR
Outcome Assessment	11. Outcome Assessment Methodology	Not rated	The metric is not applicable to this review article. Growth rate data were reported; however, more data may be available in primary sources.	NR	NR	NR
	12. Sampling Methods	Not rated	The metric is not applicable to this review article.	NR	NR	NR
Confounding/ Variable Control	13. Confounding Variables	Not rated	The metric is not applicable to this review article.	NR	NR	NR
	14. Outcomes Unrelated to Exposure	Not rated	The metric is not applicable to this review article.	NR	NR	NR
Data Presentation and Analysis	15. Data Reporting	Not rated	The metric is not applicable to this review article.	NR	NR	NR
	16. Statistical Methods and Kinetic Calculations	Not rated	The metric is not applicable to this review article.	NR	NR	NR
Other	17. Verification or Plausibility of Results	Not rated	The metric is not applicable to this review article.	NR	NR	NR
	18. QSAR Models	Not rated	The metric is not applicable to this review article.	NR	NR	NR
			Sum of scores:	3	4	6
High	Medium	Low	**Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:**	1.5	**Overall Score (Rounded):**	2.3
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			**Overall Quality Level:**	Low[1]

[1]This study's overall quality rating was downgraded. Rationale: This study is a review article with limited details reported.

Study Reference:	Janssen, DB; Jager, D; Witholt, B. (1987). Degradation of n-haloalkanes and alpha, omega-dihaloalkanes by wild-type and mutants of Acinetobacter sp. strain GJ70. Appl Environ Microbiol 53: 561-566. HERO ID: 2228540					
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 common name, 1-bromopropane.	1	2	2
	2. Test Substance Purity	High	Reported >97% purity of chlorinated and brominated compounds.	1	1	1
Test Design	3. Study Controls	High	Sterile controls were used and removed the possibility of external influences impacting the outcome.	1	2	2
	4. Test Substance Stability	High	This metric met the criteria for high confidence as expected for this type of study.	1	1	1
Test Conditions	5. Test Method Suitability	High	Halide release was measured via colorimetric assay. Haloalkane and associated alcohols of degradation were measured via GC-FID.	1	1	1

	6. Testing Conditions	High	Aerobic conditions were reported. Oxygen consumption was measured with a Clark-type oxygen electrode. pH was reported to be 7.5.	1	2	2
	7. Testing Consistency	High	Testing conditions were monitored, reported, and appropriate for the method; no conditions other than the test substance varied between tests.	1	1	1
	8. System Type and Design	High	This metric met the criteria for high confidence as expected for this type of study.	1	1	1
Test Organisms	9. Test Organism Degradation	Medium	Inoculum source was reported except for the adaptation. Not likely to have had a substantial impact on the results.	2	2	4
	10. Test Organism Partitioning	Not rated	The metric is not applicable to this study type.	NR	NR	NR
Outcome Assessment	11. Outcome Assessment Methodology	High	Degradation was measured via halide release and final concentration measurements of the substrate haloalkane and the formation of the corresponding alcohol was measured.	1	1	1

	12. Sampling Methods	High	Half-life was not reported. The amount of halide produced and the final concentration of the substrate haloalkane were measured after 6 days of incubation, which was sufficient for determining the ability of the bacteria to degrade the compounds.	1	1	1
Confounding/ Variable Control	13. Confounding Variables	Medium	Minimal discussion or report of uncertainties. Most likely did not affect outcome assessment, especially since rate constants were not being reported.	2	1	2
	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	High	Transformation products were reported. Recovery of halides was reported. Sterile controls provided sufficient evidence that disappearance of parent compound was due to the presence of the bacteria.	1	2	2
	16. Statistical Methods and Kinetic Calculations	Not rated	No kinetic calculations were done.	NR	NR	NR

Other	17.Verification or Plausibility of Results	High	This metric met the criteria for high confidence as expected for this type of study.	1	1	1
	18. QSAR Models	Not rated	The metric is not applicable to this study type.	NR	NR	NR
			Sum of scores:	16	19	22
High	Medium	Low	**Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:**	1.16	**Overall Score (Rounded):**	1.2
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			**Overall Quality Level:**	High

Study Reference:	**Sakuratani, Y; Yamada, J; Kasai, K; Noguchi, Y; Nishihara, T. (2005). External validation of the biodegradability prediction model CATABOL using data sets of existing and new chemicals under the Japanese Chemical Substances Control Law. 16: 403-431. http://dx.doi.org/10.1080/10659360500320289** **HERO ID: 2990985**					
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	Low	The source and purity of the test substance in the experimental study being compared were not reported or verified by analytical means.	3	1	3
Test Design	3. Study Controls	Not rated	The study did not require concurrent control groups.	NR	NR	NR
	4. Test Substance Stability	Medium	The test substance stability, homogeneity, preparation and storage conditions were not reported; however, these factors were not likely to have influenced the test substance or were not likely to have had a substantial impact on the study 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	There were omissions in the reporting of testing conditions; however, this was not likely to have had a substantial impact on the results.	2	2	4
	7. Testing Consistency	Not rated	The metric is not applicable to this study type (modeling).	NR	NR	NR
	8. System Type and Design	Not rated	The metric is not applicable to this study type (modeling).	NR	NR	NR
Test Organisms	9. Test Organism Degradation	Medium	Limited detail; however, the method for biodegradation was a guideline study and routinely used for similar study types and appropriate.	2	2	4
	10. Test Organism Partitioning	Not rated	The metric is not applicable to this study type (biodegradation).	NR	NR	NR
Outcome Assessment	11. Outcome Assessment Methodology	High	The experimental method and model were suitable for biodegradation assessment.	1	1	1
	12. Sampling Methods	Not rated	The metric is not applicable to this study type (modeling).	NR	NR	NR
Confounding/ Variable Control	13. Confounding Variables	Not rated	No confounding variables were noted.	NR	NR	NR
	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 data were not reported and may be available from referenced sources, but omissions were unlikely to substantially impact the results.	2	2	4
	16. Statistical Methods and Kinetic Calculations	Medium	Details for the prediction model were general.	2	1	2
Other	17. Verification or Plausibility of Results	Medium	Model validation results were low for 1-bromopropane.	2	1	2
	18. QSAR Models	Medium	This metric met the criteria for high confidence as expected for this type of study.	2	1	2
			Sum of scores:	20	15	27
High	Medium	Low	**Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:**	1.8	**Overall Score (Rounded):**	1.8
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			**Overall Quality Level:**	Medium

Study Reference:	Shochat, E; Hermoni, I; Cohen, Z; Abeliovich, A; Belkin, S. (1993). Bromoalkane-degrading Pseudomonas strains. Appl Environ Microbiol 59: 1403-1409. HERO ID: 4140374					
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 common name, 1-bromopropane.	1	2	2
	2. Test Substance Purity	Medium	The test substance source was not reported; however, the omissions were not likely to have had a substantial impact on the study results.	2	1	2
Test Design	3. Study Controls	High	The study tested a bromoalkane emulsification in aqueous medium with varying concentrations of bacteria, including a sterile control, which showed no emulsification activity.	1	2	2
	4. Test Substance Stability	High	Detailed preparation of the test substance was outlined in the methodology.	1	1	1

Test Conditions	5. Test Method Suitability	Medium	Initial 1-bromopropane concentration was not reported for the dehalogenation assays, although its omission was not likely to have impacted the results. 1- Bromooctane concentration was reported to be ca.	2	1	2
			10 - ca. 20 mmol/L so if 1-bromopropane was used in similar concentrations, it would be below its aqueous solubility of 2,450 mg/L (19,910 µmol/L).			
	6. Testing Conditions	High	Conditions were adequately monitored and reported.	1	2	2
	7. Testing Consistency	High	Every substrate was tested under the same conditions.	1	1	1
	8. System Type and Design	High	This metric met the criteria for high confidence as expected for this type of study.	1	1	1
Test Organisms	9. Test Organism Degradation	High	Inoculum source reported and concentration of cells used in each assay reported ($2x10^8$ cells per mL).	1	2	2
	10. Test Organism Partitioning	Not rated	The metric is not applicable to this study type.	NR	NR	NR

Outcome Assessment	11. Outcome Assessment Methodology	Medium	The outcome assessment was appropriate for this study but limited; the transformation products of 1-bromopropane were not identified or quantified.	2	1	2
	12. Sampling Methods	High	Sampling methods were sufficient for monitoring the outcome of interest (Br- release specifically).	1	1	1
Confounding/ Variable Control	13. Confounding Variables	High	Standard deviation was reported for some assays and no uncertainties were expected to have affected the outcome assessment.	1	1	1
	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	High	This metric met the criteria for high confidence as expected for this type of study.	1	2	2
	16. Statistical Methods and Kinetic Calculations	High	Determination of Br- release rate was done using triplicate assays and the authors reported a standard error of only 15%.	1	1	1
Other	17. Verification or Plausibility of Results	Not rated	Due to limited information, evaluation of the reasonableness of the study results was not possible.	NR	NR	NR

	18. QSAR Models	Not rated	The metric is not applicable to this study type.	NR	NR	NR
			Sum of scores:	17	19	22
High	Medium	Low	**Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:**	1.16	**Overall Score (Rounded):**	1.2
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			**Overall Quality Level:**	High

Study Reference:	Mabey, W; Mill, T. (1978). Critical review of hydrolysis of organic compounds in water under environmental conditions [Review]. J Phys Chem Ref Data 7: 383-415. HERO ID: 9848					
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 abbreviated name.	1	2	2
	2. Test Substance Purity	Medium	Substance purity was not reported but may be retrievable from referenced article.	2	1	2
Test Design	3. Study Controls	Medium	Control group information was not reported in this study but may be retrievable from referenced article.	2	2	4
	4. Test Substance Stability	Medium	Storage condition was not reported but may be retrievable from referenced article.	2	1	2
Test Conditions	5. Test Method Suitability	Medium	The test method was not reported but may be retrievable from the referenced article.	2	1	2
	6. Testing Conditions	Medium	The testing conditions were not reported but may be retrievable from the referenced article	2	2	4

	7. Testing Consistency	Medium	Testing consistency could not be determined from this study but may be retrievable from the referenced article.	2	1	2

	8. System Type and Design	Medium	More details may be retrievable from the referenced article.	2	1	2
Test Organisms	9. Test Organism Degradation	NR	The metric is not applicable to this study type.	NR	NR	NR
	10. Test Organism Partitioning	NR	The metric is not applicable to this study type.	NR	NR	NR
Outcome Assessment	11. Outcome Assessment Methodology	Medium	The outcome assessment methodology could not be evaluated from this study but reviewing the referenced article would most likely provide relevant information.	2	1	2
	12. Sampling Methods	Medium	Sampling methods could not be evaluated without reviewing the referenced article in which the hydrolysis rate was reported.	2	1	2
Confounding/ Variable Control	13. Confounding Variables	High	Values for kh estimated in section 5 at 298K are probably not more accurate than a factor of 2 (+/- 100%) or less accurate than a factor of 5 (+/- 250%) owing to uncertainties in pH, temperature	1	1	1

			coefficients, and, in some cases, solvent effects.			
	14. Outcomes Unrelated to Exposure	NR	The metric is not applicable to this study type.	NR	NR	NR
Data Presentation and Analysis	15. Data Reporting	Medium	Whether the degradation was due to another process could not be	2	2	4

			evaluated in this study.			
	16. Statistical Methods and Kinetic Calculations	High	Calculations to derive the rate constant and half-life at 298K and pH 7 were clearly outlined.	1	1	1
Other	17. Verification or Plausibility of Results	Medium	Calculated hydrolysis rates and half-lives at 298 K and pH 7 were extrapolated from measured hydrolysis rates reported in other references. However, full experimental details were not available for all studies. The authors (W. Mabey and T. Mill) are reputable sources and describe measures taken to exclude studies of questionable value.	2	1	2
	18. QSAR Models	NR	The metric is not applicable to this study type.	NR	NR	NR
			Sum of scores:	25	18	32
High	Medium	Low	**Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:**	1.7	**Overall Score (Rounded):**	1.8
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			**Overall Quality Level:**	Medium

Study Reference:	U.S. EPA (U.S. Environmental Protection Agency). (2012). Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11 [Computer Program]. Washington, DC. Retrieved from https://www.epa.gov/tsca-screening-tools/epi-suite[tm]-estimation-program- interface 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.	NR	NR	NR
	10. Test Organism Partitioning	Not rated	The metric is not applicable to this study type.	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.	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
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^{TM} have defined endpoints. Chemical domain and performance statistics for each model are known, and unambiguous algorithms are available in the EPI Suite^{TM} documentation and/or cited references to establish their scientific validity. Many EPI Suite^{TM} models have correlation coefficients >0.7, cross-validated correlation coefficients >0.5, and standard error values <0.3; however, correlation coefficients (r^2, q^2) 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	1

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:	Burkholder, JB; Gilles, MK; Gierczak, T; Ravishankara, AR. (2002). The atmospheric degradation of 1-bromopropane (CH3CH2CH2Br): The photochemistry of bromoacetone. Geophys Res Lett 29: 1822. http://dx.doi.org/10.1029/2002GL014712 HERO ID: 1733974					
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, 1-bromoacetone, was a major degradant of 1-bromopropane.	1	2	2
	2. Test Substance Purity	Medium	The test substance source and purity were not reported.	2	1	2
Test Design	3. Study Controls	Medium	Study controls were not reported; however, the lack of data was not likely to have a substantial impact on study results.	2	2	4
	4. Test Substance Stability	Not rated	The metric is not applicable to this study type.	NR	NR	NR
Test Conditions	5. Test Method Suitability	High	This metric met the criteria for high confidence as expected for this type of study.	1	1	1
	6. Testing Conditions	High	This metric met the criteria for high confidence as expected for this type of study.	1	2	2
	7. Testing Consistency	Medium	No repeated experiments were done to check for accuracy; however, this was not likely to have had a substantial impact on the study results.	2	1	2
	8. System	High	This metric met the	1	1	1

	Type and Design		criteria for high confidence as expected for this type of study.			
Test Organisms	9. Test Organism Degradation	Not rated	The metric is not applicable to this study type.	NR	NR	NR
	10. Test Organism Partitioning	Not rated	The metric is not applicable to this study type.	NR	NR	NR
Outcome Assessment	11. Outcome Assessment Methodology	High	This metric met the criteria for high confidence as expected for this type of study.	1	1	1
	12. Sampling Methods	Medium	Sampling intervals were not reported but their omission was not likely to have influenced the results.	2	1	2
Confounding/ Variable Control	13. Confounding Variables	High	Sources of variability and uncertainty in the measurements were accounted for in data evaluation.	1	1	1
	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	High	Concentrations of both target chemical and transformation products were reported.	1	2	2
	16. Statistical Methods and Kinetic Calculations	Medium	Kinetic calculations for loss rate coefficients were not clearly described but their absence was not likely to have influenced the results.	2	1	2
Other	17. Verification or Plausibility of Results	High	This metric met the criteria for high confidence as expected for this type of study.	1	1	1

	18. QSAR Models	Not rated	The metric is not applicable to this study type.	NR	NR	NR
			Sum of scores:	18	17	23
High	Medium	Low	**Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:**	1.35	**Overall Score (Rounded)**	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			**Overall Quality Level:**	High