

Office of Chemical Safety and Pollution Prevention

Revised Draft Risk Evaluation for C.I. Pigment Violet 29 (Anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone)

Systematic Review Supplemental File:

Data Quality Evaluation of Physical and Chemical Property Studies

CASRN: 81-33-4

October 2020

This document is a compilation of tables for the data extraction and evaluation for C.I. Pigment Violet 29 (CASRN 81-33-4). 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* U.S. EPA (2018). 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.

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Table 1. Melting Point Study for C.I. Pigment Violet 29

Study Reference:	BASF. 2013. Physical-Chemical properties of "Paliogen Violet 5011". BASF Study No. 11L00105. Competence Center Analytics, BASF SE, D-67056 Ludwigshafen. Test Completion Date: November 28, 2011. HERO ID: 4731544		
Note:	BASF (2013) reported various physical-chemical properties and only the confidence of the melting point is evaluated here.		
Domain/Metric	Description/ Definition	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comment
Representativeness	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance.
Evaluation/ Review	The information or data reported has reliable review.	Medium	The data is from a source that is not described as poor-reviewed by experts in the field or are broadly available to the public for review and use but is known. EPA plans to refine the criteria to clearly indicate the circumstances would make the data source to be of medium confidence for this domain/metric.
Reliability/ Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	High	The methodology is designed to determine the endpoint of interest.
Reliability/ Analytic Method	The information or data reported is from a reliable method.	High	The study used a standard and generally accepted method for this type of study.
	Overall Quality Level		High

Table 2. Log Kow Study for C.I. Pigment Violet 29

Study Reference:	BASF. 2013. Physical-Chemical properties of "Paliogen Violet 5011". BASF Study No. 11L00105. Competence Center Analytics, BASF SE, D-67056 Ludwigshafen. Test Completion Date: November 28, 2011. HERO ID: 4731544		
Note:	BASF (2013) reported various physical-chemical properties and only the confidence of the Log Kow (octanol/water partition coefficient) is evaluated here.		
Domain/Metric	Description/ Definition	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comment
Representativeness	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	Unacceptable	The substance is not soluble in either octanol or water. Therefore, partitioning between the media cannot be determined.
Evaluation/ Review	The information or data reported has reliable review.	Medium	The data is from a source that is not described as poor-reviewed by experts in the field or are broadly available to the public for review and use, but is known. EPA plans to refine the criteria to clearly indicate the circumstances would make the data source to be of medium confidence for this domain/metric.
Reliability/ Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	Not Rated	Data source does not provide information to determine the method objectivity (unbiased method). Thus the domain/ metric was not rated.
Reliability/ Analytic Method	The information or data reported is from a reliable method.	Unacceptable	The substance is not soluble in either octanol or water. Therefore, partitioning between the media cannot be determined. This analytical method is not appropriate.
	Overall Quality Level		Unacceptable

Table 3. Density Study for C.I. Pigment Violet 29

Study Reference:	BASF. 2013. Physical-Chemical properties of "Paliogen Violet 5011". BASF Study No. 11L00105. Competence Center Analytics, BASF SE, D-67056 Ludwigshafen. Test Completion Date: November 28, 2011.		
Note:	BASF (2013) reported the relative density of PV-29.		
Domain/Metric	Description/ Definition	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comment
Representativeness	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance.
Evaluation/ Review	The information or data reported has reliable review.	Medium	From a source, Competence Center Analytics, BASF SE, D-67056 Ludwigshafen, that is not described as High, but is known; where High corresponds to a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use, and include references to the original sources.
Reliability/ Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	High	The methodology is designed to determine the endpoint of interest.
Reliability/ Analytic Method	The information or data reported is from a reliable method.	High	The study used a standard and generally accepted method for this type of study.
	Overall Quality Level		High

Table 4. Vapor Pressure Study for C.I. Pigment Violet 29

Study Reference:	BASF. 2013. Physical-Chemical properties of "Paliogen Violet 5011". BASF Study No. 11L00105. Competence Center Analytics, BASF SE, D-67056 Ludwigshafen. Test Completion Date: November 28, 2011.		
Note:	BASF (2013) reported the vapor pressure of PV-29.		
Domain/Metric	Description/ Definition	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comment
Representativeness	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance.
Evaluation/ Review	The information or data reported has reliable review.	Medium	From a source, Competence Center Analytics, BASF SE, D-67056 Ludwigshafen, that is not described as High, but is known; where High corresponds to a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use, and include references to the original sources.
Reliability/ Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	High	The methodology is designed to determine the endpoint of interest.
Reliability/ Analytic Method	The information or data reported is from a reliable method.	High	The study used a standard and generally accepted method for this type of study; however, a cutoff value was reported because the limit of the most sensitive measurement technique was reached.
	Overall Quality Level		High

Table 5. Solubility in n-Octanol Study for C.I. Pigment Violet 29

Study Reference:	Sun Chemical. 2020. Determination of the solubility of C.I. PV29 in 1-octanol and water. Sun Chemical Study No. 04-033A-WOS. Colors Technology Analytical Laboratory, Sun Chemical Corporation, 5020 Spring Grove Avenue, Cincinnati Ohio 45232. Test Completion Date: Original: June 1, 2020; Revised: June 22, 2020.		
Note:	Sun Chemicals (2020) reported the solubility in n-octanol of PV-29.		
Domain/Metric	Description/ Definition	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comment
Representativeness	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance (high melting solid). It should be noted that the company reported no physical evidence of any solubility; therefore, they reported values were for the LOD (0.0014 mg/L) and the LOQ (0.003 mg/L).
Evaluation/ Review	The information or data reported has reliable review.	Medium	From a source, Colors Technology Analytical Laboratory, Sun Chemical Corporation that is not described as High, but is known; a High determination corresponds to a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use, and include references to the original sources.
Reliability/ Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	High	The methodology is designed to determine the endpoint of interest. The company used a method which was agreed upon at the "Analytical Experts Meeting" of ETAD (Basel) on January 12, 2005. Due to the substance's low solubility in all solvents, other methods could not be used.
Reliability/ Analytic Method	The information or data reported is from a reliable method.	High	The study used a generally accepted method for this type of study; however, a cutoff value was reported since the test substance solubility in n-octanol was below the limit of quantification and most likely below the limit of detection.
	Overall Quality Level		High

Table 6. Solubility in Water Study for C.I. Pigment Violet 29

Study Reference:	Sun Chemical. 2020. Determination of the solubility of C.I. PV29 in 1-octanol and water. Sun Chemical Study No. 04-033A-WOS. Colors Technology Analytical Laboratory, Sun Chemical Corporation, 5020 Spring Grove Avenue, Cincinnati Ohio 45232. Test Completion Date: Original: June 1, 2020; Revised: June 22, 2020.			
Note:	Sun Chemicals (2020) repo	Sun Chemicals (2020) reported the solubility in water of PV-29.		
Domain/Metric	Description/ Definition	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comment	
Representativeness	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.	
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance (high melting solid). It should be noted that the company reported no physical evidence of any solubility; therefore, they reported values were for the LOD (0.0014 mg/L) and the LOQ (0.003 mg/L).	
Evaluation/ Review	The information or data reported has reliable review.	Medium	From a source, Colors Technology Analytical Laboratory, Sun Chemical Corporation that is not described as High, but is known; a High determination corresponds to a recognized data collection/repository where data are peer- reviewed by experts in the field, are broadly available to the public for review and use, and include references to the original sources.	
Reliability/ Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	High	The methodology is designed to determine the endpoint of interest. The method was based on the OECD 105 flask method. Due to the substance's low solubility in all solvents, other methods could not be used.	
Reliability/ Analytic Method	The information or data reported is from a reliable method.	High	The study used a generally accepted method for this type of study; however, a cutoff value was reported since the test substance solubility in water was below the limit of quantification and most likely below the limit of detection.	
	Overall Quality Level		High	

References

- <u>BASF.</u> (2013). Physical-chemical properties of "Paliogen violet 5011". BASF study no. 11L00105. (11L00105). Ludwigshafen: Competence Center Analytics; BASF SE; D-67056.
- <u>Sun Chemicals.</u> (2020). Enclosure 1 EPA request for additional information in response to SACC peer reveiwer and including public comments on the draft C.I. Pigment Violet 20 Risk Evaluation.
- <u>U.S. EPA.</u> (2018). Application of systematic review in TSCA risk evaluations. (740-P1-8001). Washington, DC: U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention. https://www.epa.gov/sites/production/files/2018-06/documents/final_application_of_sr_in_tsca_05-31-18.pdf.