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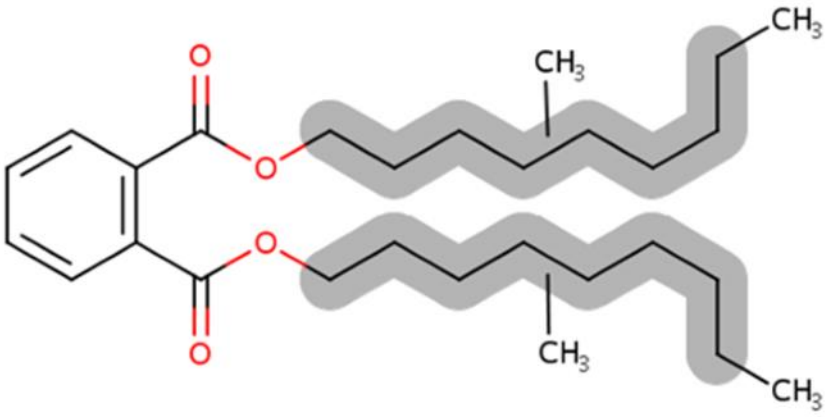
Pollution Prevention

Physical Chemistry Assessment for Diisodecyl Phthalate (DIDP)

Technical Support Document for the Risk Evaluation

CASRNs: 26761-40-0 and 68515-49-1



(Representative Structure)

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TABLE OF CONTENTS

LIST OF TABLES

KEY ABBREVIATIONS AND ACRONYMS

Atm	Atmospheres
$atm \cdot m^3/mol$	Atmospheres - cubic meters per mole
C	Celsius
CASRN	Chemical abstract service registry number
cP	Centipoise
DIDP	Diisodecyl phthalate
EPA	Environmental Protection Agency (U.S.)
F	Fahrenheit
g/cm^3	Grams per cubic centimeter
HSDB	Hazard Substance Data Bank
K	Kelvin
K_{OA}	Octanol-air partition coefficient
K_{OW}	Octanol-water partition coefficient
Mg/L	Milligrams per liter
mol	Mole
mmHG	Millimeters of mercury
NLM	National Library of Medicine
Pa (hPa)	Pascals (hectopascals; 1 hPa = 100 Pa)
SVOC	Semi-volatile organic compound

SUMMARY

This technical document is in support of the TSCA *Risk Evaluation for Diisodecyl Phthalate (DIDP)* (U.S. EPA, 2024b). DIDP is a common chemical name for the category of chemical substances that includes the following substances: 1,2-benzenedicarboxylic acid, 1,2-diisodecyl ester (CASRN 26761-40-0) and 1,2-benzenedicarboxylic acid, di-C9-11-branched alkyl esters, C10-rich (CASRN 68515-49-1). Both CASRNs contain mainly C10 dialkyl phthalate esters. See the risk evaluation for a complete list of all the technical support documents for DIDP.

In this document, EPA gathered and evaluated physical and chemical property data and information according to the process described in the *Systematic Review Protocol for Diisodecyl Phthalate (DIDP)* (U.S. EPA, 2024c). During the evaluation of DIDP, EPA considered both measured and estimated physical and chemical property data/information summarized in Table 2-1, as applicable. Information on the full, extracted data set is available in the *Data Quality Evaluation and Data Extraction Information for Physical and Chemical Properties for Diisodecyl Phthalate (DIDP)* (U.S. EPA, 2024a).

DIDP is a clear, oily, viscous, transparent liquid with a mild odor (HSDB, 2015). As a branched phthalate ester, DIDP is used as plasticizer that melts around −50 °C (Haynes, 2014). DIDP is considered insoluble in water with water solubility of 0.00017 mg/L at 20 °C and a high log K_{OW} (10.21) (ECCC/HC, 2020; U.S. EPA, 2017; Letinski et al., 2002). With a vapor pressure of 5.28×10^{-7} mmHg at 25 °C (NLM, 2020) and a boiling point of greater than 400 °C (Haynes, 2014), DIDP has low volatility and is categorized as a semi-volatile organic compound (SVOC) (ECCC/HC, 2020), and has a Henry's Law coefficient of 2.132×10^{-4} atm·m^3/mol at 25 °C (Cousins and Mackay, 2000).

1 INTRODUCTION

DIDP is produced by the esterification of phthalic anhydride with isodecanol. Commercially, DIDP is not a single compound but rather a complex mixture of phthalate esters having branched alkyl chains with an average chain length of 10. The following sections discuss the selection of the physical and chemical properties of DIDP.

2 EVIDENCE INTEGRATION FOR PHYSICAL AND CHEMICAL PROPERTIES

Due to the relative availability of data, only studies with an overall data quality determination of High and Medium were selected for use in determining the representative physical and chemical properties of DIDP for the purposes of the risk evaluation.

2.1 Final Selected Physical and Chemical Property Values for DIDP

Table 2-1. Summary of Physical and Chemical Property Values for DIDP

Property	Selected Value	Reference	Overall Quality Determination
Molecular formula	$C_{28}H_{46}O_4$		
Molecular weight	446.7 g/mol		
Physical form	Clear Liquid	(Haynes, 2014)	High
Melting point	−50 °C	(Haynes, 2014)	High
Boiling point	>400 °C	(Haynes, 2014)	High
Density	0.967 g/cm^3 at 25 °C	(Cadogan and Howick, 2000)	High
Vapor pressure	5.28E-07 mmHg at 25 °C	(NLM, 2020)	High
Vapor density	15.4 (air = 1)	(NLM, 2020)	High
Water solubility	0.00017 mg/L at 20 °C	(Letinski et al., 2002)	High
Octanol:water partition coefficient (log K_{OW})	10.21 (EPI Suite™)	(U.S. EPA, 2017)	High
Octanol:air partition coefficient (log K_{OA})	13.0 (EPI Suite™)	(U.S. EPA, 2017)	High
Henry's Law constant	2.132E−04 atm·m^3/mol at 25 °C	(Cousins and Mackay, 2000)	High
Flash point	>200 °C	(ECJRC, 2003)	High
Autoflammability	402 °C	(NLM, 2020)	Medium
Viscosity	87.797 cP at 20 °C	(Caetano et al., 2005)	High

2.2 Endpoint Assessments

2.2.1 Melting Point

The EPA extracted and evaluated eleven sources containing DIDP melting point information. Five of the sources were identified and evaluated as overall high-quality data sources and the remaining six as overall medium-quality data sources. The overall high-quality sources reported DIDP melting points ranging from −50 to −45 °C (NLM, 2020; U.S. EPA, 2019; Haynes, 2014; NTP-CERHR, 2003; Park and Sheehan, 2000). EPA selected a melting point value of –50 ± 1.97 °C (Haynes, 2014) as a representative value of the available information obtained from the overall high-quality data sources. In addition, the selected value is consistent with the value selected in the *Final Scope of the Risk*

Evaluation for Di-isodecyl Phthalate (DIDP), CASRN 26761-40-0 and 68515-49-1 (Final Scope for the Risk Evaluation of DIDP) (U.S. EPA, 2021).

2.2.2 Boiling Point

The EPA extracted and evaluated ten data sources containing DIDP boiling point information. Five of the sources were identified and evaluated as overall high-quality data sources and the remaining five as overall medium-quality data sources. The overall high-quality sources reported DIDP boiling points ranging from 250 to 370 °C (NLM, 2020; Haynes, 2014; ECJRC, 2003; NTP-CERHR, 2003; Park and Sheehan, 2000). EPA selected a boiling point value of greater than 350 °C (NTP-CERHR, 2003) as a representative value under normal environmental conditions within the available information obtained from the overall high-quality data sources.

2.2.3 Density

The EPA extracted and evaluated 17 data sources containing DIDP density information. Twelve of the sources were identified and evaluated as overall high-quality data sources and the remaining five as overall medium-quality data sources. The overall high-quality sources reported DIDP density values ranging from 0.961 to 0.97 g/cm^3 (NLM, 2020; HSDB, 2015; Haynes, 2014; Brito e Abreu et al., 2010; Peleties et al., 2010; Paredes et al., 2009; Harris and Bair, 2007; Caetano et al., 2006; Caetano et al., 2005; NTP-CERHR, 2003; Cadogan and Howick, 2000; Park and Sheehan, 2000). EPA selected a density of 0.967 g/cm^3 (Cadogan and Howick, 2000) to represent the most prevalent value at 298.15 K within the available information obtained from the overall high-quality data sources. This value has replaced the value selected in the Final Scope for the Risk Evaluation of DIDP (U.S. EPA, 2021) of 0.9634 g/cm^3 at 293.15 K (Brito e Abreu et al., 2010).

2.2.4 Vapor Pressure

The EPA extracted and evaluated seven data sources containing DIDP vapor pressure information. Four of the sources were identified and evaluated as overall high-quality data sources and the remaining three as overall medium-quality data sources. These sources reported DIDP vapor pressure ranging from 1.38×10^{-8} to 5.28×10^{-7} mmHg (ECCC/HC, 2020; NLM, 2020; EC/HC, 2015; ECHA, 2013; Lu, 2009; Cousins et al., 2007; ECJRC, 2003). EPA selected a vapor pressure value of 5.28×10^{-7} mmHg (NLM, 2020) as a representative value of the available information obtained from the overall medium and high-quality data sources under normal environmental conditions. In addition, the selected value is consistent with the value selected in the Final Scope for the Risk Evaluation of DIDP (U.S. EPA, 2021).

2.2.5 Vapor Density

A value for vapor density was not identified in the initial data review for the Final Scope for the Risk Evaluation of DIDP (U.S. EPA, 2021). Systematic review identified a single overall high-quality study which indicated a vapor density of 15.4 (air = 1) for DIDP (NLM, 2020).

2.2.6 Water Solubility

Water solubility informs many endpoints not only within the realm of fate and transport of DIDP in the environment, but also informs endpoints and data quality and modelling decisions in industrial processes and engineering, and human and ecological hazards and exposure. A systematic review of reasonably available data on the water solubility of DIDP was conducted. The EPA extracted and evaluated twelve data sources containing DIDP water solubility information. Seven of the sources were identified and evaluated as overall high-quality data sources and the remaining five as overall medium-quality data sources. During examination, many methods used a shake flask or continuous stirring method which has been shown in high molecular weight phthalates to cause colloidal suspensions of small amounts of free product in solution. These suspensions are stable and attempts to determine analytically may lead to

erroneously high measurements of true solubility for DIDP. As a result, water solubility measurements obtained in these tests may exceed the true water solubility of DIDP. However, Letinski (2002) reported DIDP water solubility of 0.00017 mg/L in a slow stir method designed to minimize the presence of colloidal suspensions. Water solubility values collected in the systematic review process for DIDP exhibited a range of values from 0.00017 to 1.19 mg/L (ECCC/HC, 2020; NLM, 2020; ECJRC, 2003; NTP-CERHR, 2003; Letinski et al., 2002; Howard et al., 1985; SRC, 1983). A representative value of 0.00017 mg/L was selected for use in the risk evaluation (Letinski et al., 2002).

2.2.7 Log Octanol/Water Partitioning Coefficient

The EPA extracted and evaluated eight data sources containing DIDP octanol-water partition coefficient information. Two of the sources were identified and evaluated as overall high-quality data sources and the remaining six as overall medium-quality data sources. These sources reported DIDP log K_{OW} ranging from 8.8 to 10.36 (RSC, 2019; EC/HC, 2015; U.S. CPSC, 2015; ECHA, 2013; Lu, 2009; Cousins et al., 2007; NTP-CERHR, 2003, 2000). The octanol partitioning coefficient originally selected in the Final Scope for the Risk Evaluation of DIDP (log K_{OW} = 10.352) (U.S. EPA, 2021) was reported by the Royal Society of Chemistry in PubChem but has since been removed from the database. One of the overall high-quality data sources reported a log K_{OW} of ~10 but did not list whether it was experimentally derived, calculated, or modelled (NTP-CERHR, 2003). The second high-quality data source reported a model estimated log K_{OW} value of 10.352 (RSC, 2019). The EPA selected an EPI Suite™ predicted modelled value for log K_{OW} of 10.21, to represent the average within the high-quality data sources, in the risk assessment (U.S. EPA, 2017).

2.2.8 Henry's Law Constant

The Henry's Law Constant selected in the Final Scope for the Risk Evaluation of DIDP (U.S. EPA, 2021) was a value calculated in EPI Suite™ from the vapor pressure and water solubility of DIDP and was 1.1×10^{-6} atm-m^3 /mole at 25°C EPI Suite™ (U.S. EPA, 2012). One overall high-quality and two overall medium studies were identified in the systematic review process for DIDP, ranging from 2.13×10^{-4} to 1.13×10^{-3} atm-m^3 /mole (ECHA, 2013; Cousins et al., 2007; Cousins and Mackay, 2000). The resulting selected value for use in the risk evaluation of DIDP is 2.132×10^{-3} atm·m^3/mol at 25 °C (Cousins and Mackay, 2000). This aligns with DIDP's designation as a semi-volatile organic compound (SVOC) (EC/HC, 2015).

2.2.9 Flashpoint

A value for the flashpoint of DIDP was selected to be 232 °C (RSC, 2019) in the initial data review for the Final Scope for the Risk Evaluation of DIDP (U.S. EPA, 2021). After the systematic review process, this study received a data quality ranking of medium. The systematic review process identified a several overall high-quality references that indicated a flashpoint of greater than 200 °C for DIDP (ECJRC, 2003), which was used in place of the medium quality data point utilized in the scoping stage.

2.2.10 Autoflammability

A value for the automatability of DIDP was not identified in the initial data review for the Final Scope for the Risk Evaluation of DIDP (U.S. EPA, 2021). The systematic review process identified several overall medium-quality references reporting autoflammability values ranging from 365 to 402 °C (NLM, 2020; ECHA, 2013; ECJRC, 2003). The EPA selected an autoflammability temperature of 402 °C for DIDP (NLM, 2020; ECHA, 2013; ECJRC, 2003)

2.2.11 Viscosity

In the Final Scope for the Risk Evaluation of DIDP (U.S. EPA, 2021). A value of 108 cP at 20 °C was identified as the viscosity for DIDP (HSDB, 2015). Several high-quality studies were identified during

the systematic review process reporting viscosity values from 85.3 to 88.7 cP (Assael and Mylona, 2013; Peleties and Trusler, 2011; da Mata et al., 2009; Al Motari et al., 5622157 5622157; Froeba and Leipertz, 2007; Harris and Bair, 2007; Caetano et al., 2006; Caetano et al., 2005, 2004; ECJRC, 2003). The EPA selected a value of 87.797 cP at 20 °C as a representative value of the mean viscosity for DIDP (Caetano et al., 2005) replacing the scoping value as it was a high-quality primary source that was experimentally derived.

2.3 Strengths, Limitations, Assumptions, and Key Sources of Uncertainty for the Physical and Chemical Property Assessment

Due to the low water solubility of DIDP, certain physical and chemical properties may be difficult to measure experimentally (water solubility, octanol/water partitioning coefficient, organic carbon partitioning coefficients) with traditional guideline tests. The selection of these values was based on professional judgement and the overall data quality ranking of the associated references. In some instances where no data were available, or there was a wide range of resorted data that generally, but did not consistently agree with one another, models such as EPI Suite™ were used to estimate the value for the endpoint (octanol water partitioning coefficient and organic carbon partitioning coefficient) and cross checked with reported data from systematic review.

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