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Draft Physical Chemistry Assessment for Diisononyl Phthalate (DINP)

Technical Support Document for the Draft Risk Evaluation

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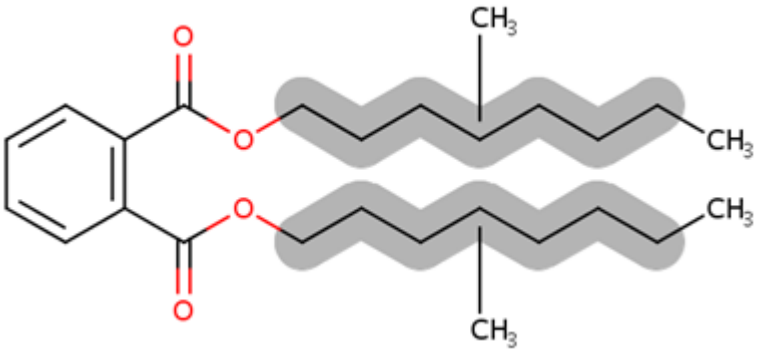

(Representative Structure)

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ABBREVIATIONS AND ACRONYMS

Atm	Atmospheres
atm·m^3/mol	Atmospheres – cubic meters per mole
C	Celsius
CASRN	Chemical Abstract Service registry number
cP	Centipoise
DIDP	Diisodecyl phthalate
DINP	Diisononyl phthalate
EPA	Environmental Protection Agency
F	Fahrenheit (°F)
g/cm^3	Grams per cubic centimeter
K	Kelvin
KOA	Octanol-air partition coefficient
KOW	Octanol-water partition coefficient
mg/L	milligrams per liter
mol	Mole
mmHg	millimeters of mercury
N/A	Not applicable
NR	Not reported
Pa (hPa)	Pascals (hectopascals; 1 hPa = 100 Pa)
RSC	Royal Society of Chemistry
SVOC	Semi-volatile organic compound

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Docket

Supporting information can be found in the public docket, Docket ID (EPA-HQ-OPPT-2024-0073).

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SUMMARY

EPA gathered and evaluated physical and chemical property data and information according to the process described in the *Draft Risk Evaluation for Diisononyl Phthalate (DINP) – Systematic Review Protocol* (U.S. EPA, 2024a). During the evaluation of DINP, EPA considered both measured and estimated physical and chemical property data/information summarized in Table 2-1, as applicable. Information on the full, extracted dataset is available in the file *Draft Risk Evaluation for Di-isononyl Phthalate (DINP) – Systematic Review Supplemental File: Data Quality Evaluation and Data Extraction Information for Physical and Chemical Properties* (U.S. EPA, 2024b).

DINP is a clear, oily, viscous liquid with a mild odor (HSDB, 2015). As a branched phthalate ester, DINP is used as plasticizer that melts around −48 °C (NCBI, 2020; RSC, 2019; NLM, 2015; O'Neil, 2013; NTP-CERHR, 2003). DINP is considered insoluble in water with water solubility of 0.00061 mg/L at 20 °C (Letinski et al., 2002) and a log K_{OW} of 8.8 (ECHA, 2016). With a vapor pressure of 5.40×10^{-7} mmHg at 25 °C (NLM, 2015) and a boiling point greater than 400 °C (ECHA, 2016), DINP has low volatility and is categorized as a semi-volatile organic compound (SVOC) (ECCC/HC, 2020). The selected Henry's Law constant for DINP was 9.14×10^{-5} atm·m^3/mol at 25 °C (Cousins and Mackay, 2000).

1 INTRODUCTION

DINP is produced by the esterification of phthalic anhydride with isononanol. Commercially, DINP is not a single compound but rather a complex mixture of phthalate esters having branched alkyl chains with an average chain length of nine. The following sections present the general physical and chemical properties of DINP.

2 EVIDENCE INTEGRATION FOR PHYSICAL AND CHEMICAL PROPERTIES

Due to the large quantity of available data, only studies with an overall data quality ranking of High were selected for use in determining the representative physical chemical properties of DINP for the purposes of the draft risk evaluation.

2.1 Final Selected Physical and Chemical Property Values for DINP

Table 2-1. Summary of DINP's Physical and Chemical Property Information

Property	Selected Value	Reference	Overall Quality Determination
Molecular formula	$C_{26}H_{42}O_4$		
Molecular weight	418.62 g/mol		
Physical form	Clear Liquid	(NLM, 2015)	High
Melting point	−48 °C	(O'Neil, 2013)	High
Boiling point	>400 °C	(ECHA, 2016)	High
Density	0.97578 g/cm^3	(De Lorenzi et al., 1998)	High
Vapor pressure	5.40E-07 mmHg	(NLM, 2015)	High
Water solubility	0.00061 mg/L	(Letinski et al., 2002)	High
Octanol:water partition coefficient (log K_{OW})	8.8	(ECHA, 2016)	High
Octanol:air partition coefficient (log K_{OA})	11.9 (EPI Suite™)	(U.S. EPA, 2017)	High
Henry's Law constant	9.14E−05 atm·m^3/mol at 25 °C	(Cousins and Mackay, 2000)	High
Flash point	213 °C	(O'Neil, 2013)	High
Autoflammability	400 °C	(ECHA, 2016)	High
Viscosity	77.6 cP	(ECHA, 2016)	High

2.2 Endpoint Assessments

2.2.1 Melting Point

The EPA extracted and evaluated 11 sources containing DINP melting point information. Five of the sources were identified and evaluated as overall high-quality data sources, four as overall medium-quality data sources, and the remaining two as overall low-quality data sources. The overall high-quality sources reported DINP melting points ranging from −48 to −43 °C (NCBI, 2020; RSC, 2019; NLM, 2015; O'Neil, 2013; NTP-CERHR, 2003). EPA selected a melting point value of −48 ± 1 °C (O'Neil, 2013) as a representative value of the identified information from the overall high-quality data sources. In addition, the identified value is consistent with the value selected in the Final Scope for the Risk Evaluation of DINP (U.S. EPA, 2021).

2.2.2 Boiling Point

The EPA extracted and evaluated 10 data sources containing DINP boiling point information. Four of

the sources were identified and evaluated as overall high-quality data sources, three as overall medium-quality data sources and the remaining three as overall low-quality data sources. The overall high-quality sources reported DINP boiling points ranging from 244 °C to greater than 400 °C (NCBI, 2020; ECHA, 2016; O'Neil, 2013; NTP-CERHR, 2003). EPA selected a boiling point value of greater than 400 °C (ECHA, 2016) as a representative value under normal environmental conditions within the identified information in the overall high-quality data sources.

2.2.3 Density

The EPA extracted and evaluated 12 data sources containing DINP density information. Seven of the sources were identified and evaluated as overall high-quality data sources, three as overall medium-quality data sources, and the remaining two as overall low-quality data sources. The overall high-quality sources reported DINP density values ranging from 0.97 to 0.98 g/cm^3 (NCBI, 2020; ECHA, 2016; NLM, 2015; O'Neil, 2013; NTP-CERHR, 2003; ExxonMobil, 2001; De Lorenzi et al., 1998). EPA selected a density of 0.97578 g/cm^3 (De Lorenzi et al., 1998) as DINP's representative density value within the identified information obtained from the overall high-quality data sources. In addition, the identified value is consistent with the value selected in the Final Scope for the Risk Evaluation of DINP (U.S. EPA, 2021).

2.2.4 Vapor Pressure

The EPA extracted and evaluated eleven data sources containing DINP vapor pressure 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 DINP vapor pressure ranging from 9.6×10^{-8} to 5.4×10^{-7} mmHg at 20 to 25 °C (ECHA, 2016; NLM, 2015; Lu, 2009; Howard et al., 1985). EPA selected a vapor pressure value of 5.40×10^{-7} mmHg (NLM, 2015) as a representative value of the identified information obtained from the overall high-quality data sources under normal environmental conditions. In addition, the identified value is consistent with the value selected in the Final Scope for the Risk Evaluation of DINP (U.S. EPA, 2021).

2.2.5 Vapor Density

A value for vapor density was not identified during systematic review or the initial data review for the Final Scope for the Risk Evaluation of DINP (U.S. EPA, 2021).

2.2.6 Water Solubility

Water solubility informs many endpoints not only within the realm of fate and transport of DINP in the environment, but also informs modelling decisions in industrial processes, engineering, human and ecological hazards, and exposure. A systematic review of reasonably available data on the water solubility of DINP was conducted. The EPA extracted and evaluated 15 data sources containing DINP water solubility information. Six of the sources were identified and evaluated as overall high-quality data sources, seven as overall medium-quality data sources, and the remaining two as overall low-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 DINP. As a result, water solubility measurements obtained in these tests may exceed the true water solubility of DINP. However, Letinski (2002) reported DINP water solubility of 0.00061 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 DINP exhibited a range of values from 0.0006 to 0.2 mg/L (ECCC/HC, 2020; ECHA, 2016; NLM, 2015; NTP-CERHR, 2003; Letinski et al., 2002; Howard et al., 1985). A representative value of 0.00061 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 13 data sources containing DINP octanol-water partition coefficient (K_{OW}) information. Five of the sources were identified and evaluated as overall high-quality data sources, seven as overall medium-quality data sources, and one as overall low-quality data sources. The overall high-quality sources reported DINP log K_{OW} ranging from 8.8 to 9.7 (ECCC/HC, 2020; ECHA, 2016; NLM, 2015; O'Neil, 2013; NTP-CERHR, 2003). EPA selected a measured read across log K_{OW} value of 8.8 (ECHA, 2016) for this risk evaluation.

2.2.8 Henry's Law Constant

The Henry's Law constant selected in the Final Scope for the Risk Evaluation of DINP (U.S. EPA, 2021) was a value calculated in EPI Suite™ from the vapor pressure and water solubility of DINP and was 2.08×10^{-5} 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 revie process for DINP, ranging from 9.14×10^{-5} to 4.09×10^{-4} atm-m^3 /mole (ECHA, 2013; Cousins et al., 2007; Cousins and Mackay, 2000). The EPA identified Henry's Law constant value of 9.14×10^{-5} atm·m^3/mol at 25 °C (Cousins and Mackay, 2000) for this risk evaluation. Based on the identified Henry's Law constant value, DINP is considered an SVOC.

2.2.9 Flashpoint

The EPA extracted and evaluated four data sources containing DINP flash point information. Three of the sources were identified and evaluated as overall high-quality data sources and one as overall medium-quality data sources. The overall high-quality sources reported DINP flash points ranging from 213 to 236 °C (NCBI, 2020; ECHA, 2016; O'Neil, 2013). EPA selected a flash point value of 213 °C (O'Neil, 2013) as a representative value of the available information identified from the overall high-quality data sources under normal environmental conditions. In addition, the identified value is consistent with the value selected in the Final Scope for the Risk Evaluation of DINP (U.S. EPA, 2021).

2.2.10 Autoflammability

A value for the automatability of DINP was not identified in the initial data review for the Final Scope for the Risk Evaluation of DINP (U.S. EPA, 2021). The systematic review process identified one overall high-quality and two overall medium-quality references reporting autoflammability values ranging from 380 to 400 °C (NCBI, 2020; ECHA, 2016, 2013). The EPA selected an autoflammability temperature of 400 °C for DINP (ECHA, 2016) for this risk evaluation.

2.2.11 Viscosity

In the Final Scope for the Risk Evaluation of DINP (U.S. EPA, 2021) a value of 55.334 cP at 25 °C was identified as the viscosity for DINP (De Lorenzi et al., 1998). Four overall high-quality data sources were identified during the systematic review process reporting viscosity values from 55.334 to 102 cP (NCBI, 2020; ECHA, 2016; NLM, 2015; De Lorenzi et al., 1998). The EPA selected a value of 77.6 cP at 20 °C as a representative value of the mode viscosity for DINP (ECHA, 2016) replacing the scoping value.

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

Due to the water solubility of DINP, 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 representative physical and chemical property values were selected 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 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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