

Eco-profiles and Environmental Product Declarations of the European Plastics Manufacturers

**Di-isononyl phthalate (DINP)** ECPI January 2015



## **Table of Content**

Table of Content
Environmental Product Declaration
Introduction4
Meta Data4
Description of the Product and the Production Process4
Environmental Performance5
Additional Environmental and Health Information5
Additional Technical Information5
Additional Economic Information5
Information6
Goal & Scope7
Intended Use & Target Audience7
Product Category and Declared Unit7
Product and Producer Description
Eco-profile – Life Cycle Inventory 10
System Boundaries10
Cut-off Rules 11
Data Quality Requirements 11
Calculation Rules13
Life Cycle Inventory (LCI) Results15
Life Cycle Impact Assessment (LCIA)
Input22
Output22
Reviews
Internal Independent Quality Assurance Statement26
External Independent Review Summary27
References 29

## List of Abbreviations

Abbreviation	Explanation
ADP	Abiotic Depletion Potential
AP	Acidification Potential
BOD	Biological Oxygen Demand
CEFIC	The European Chemical Industry Council
CFCs	Chlorofluorocarbons
CML	Centre of Environmental Science, Leiden University
COD	Chemical Oxygen Demand
DEHP	Di-2-ethylhexyl phthalate
DIDP	Di-isodecyl phthalate
DINP	Di-isononyl phthalate
ECPI	European Council for Plasticisers and Intermediates
EPD	Environmental Product Declaration
EP	Eutrophication Potential
GaBi	Ganzheitliche Bilanzierung (German for holistic balancing)
GWP	Global Warming Potential
ILCD	International Life Cycle Data System
INA	Isononanol (=Isononyl Alcohol)
ISO	International Organization for Standardization
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LHV	Lower Heating Value
ODP	Ozone Depletion Potential
PCR	Product Category Rules
PE	PE INTERNATIONAL
PM	Particulate Matter
РОСР	Photochemical Ozone Creation Potential
PVC	Polyvinyl Chloride
ТОС	Total Organic Carbon
UHV	Upper Heating Value
VOC	Volatile Organic Compound

## **Environmental Product Declaration**

### Introduction

This Environmental Product Declaration (EPD) is based upon life cycle inventory (LCI) data from PlasticsEurope's Eco-profile programme. It has been prepared according to **PlasticsEurope's Eco-profiles and Environmental Declarations – LCI Methodology and PCR for Uncompounded Polymer Resins and Reactive Polymer Precursors** (PCR version 2.0, April 2011). EPDs provide environmental performance data, but no information on the economic and social aspects which would be necessary for a complete sustainability assessment. EPDs do not imply a value judgment between environmental criteria.

This EPD describes the production of the Di-isononyl phthalate (DINP) plasticizer from cradle to gate (from crude oil extraction to product at plant, i.e. DINP production site output). **Please keep in mind that comparisons** <u>cannot</u> be made on the level of the plasticizer material alone: it is necessary to consider the full life cycle of an application in order to compare the performance of different materials and the effects of relevant life cycle parameters. This EPD is intended to be used by member companies, to support product-orientated environmental management; by users of plasticizers, as a building block of life cycle assessment (LCA) studies of individual products; and by other interested parties, as a source of life cycle information.

#### Meta Data

Data Owner	European Council for Plasticisers and Intermediates (ECPI)
LCA Practitioner	PE INTERNATIONAL AG
Programme Owner	PlasticsEurope aisbl
Programme Manager	DEKRA Consulting GmbH
LCA Reviewer	denkstatt GmbH
Number of plants in- cluded in data collec- tion	3
Representativeness	90%
Reference year	2011
Year of data collection and calculation	2014
Expected temporal va- lidity	2019
Cut-offs	No significant cut-offs
Data Quality	Good
Allocation method	Price allocation

## Description of the Product and the Production Process

Di-isononyl phthalate (DINP) is an oily colourless liquid with a slight ester odour.

#### **Production Process**

Di-isononyl phthalate is produced by one-step esterification of phthalic anhydride with isononanol (INA) and a catalyst. Two types of isononanol can be used for the synthesis: either a pure C9 fraction (synthesized from isooctene), or a C8-C10 fraction, C9-rich (synthesized from C7-C9, C8-rich alkene). The reference flow to which all data given in this EPD refer is 1 kg of DINP.

#### **Data Sources and Allocation**

The main data source was a primary data collection from European producers of DINP, providing sitespecific gate-to-gate production data for processes under operational control of the participating companies: three DINP producers with three plants in two different European countries. This covers 90% of the European DINP production capacity (EU-27) in 2011. The data for the upstream supply chain until the precursors are modelled from literature sources or are taken from the database of the software system GaBi 6 [GABI 6 2013]. One company additionally delivered primary data for the production of the precursor isononanol. Two different routes for the production of isooctene, the precursor of isononanol, were modelled as per the actual supply situation: butene dimerization and the polygas route. All relevant background data, such as energy generation and auxiliary materials, are from the GaBi 6 database, but are also publicly available and documented [GABI 6 2013]. Price allocation was applied where co-products of DINP production were relevant.

#### **Use Phase and End-of-Life Management**

DINP is used as a general, all-purpose plasticizer, 95% of which is used in PVC applications such as wire and cables, flooring, truck tarpaulins, wall covering, self-adhesive films or labels, synthetic leather, coated fabrics, technical foils, roofing membranes and automotive applications. More than half of the DINP used in non-PVC applications involves polymer related-uses (e.g. rubbers). The remaining DINP is used in inks and pigments, adhesives, sealants, paints and lacquers and lubricants (ECPI 2014). At the end of life PVC products containing DINP are either recycled for similar applications, landfilled or incinerated.

## **Environmental Performance**

The tables below show the environmental performance indicators associated with the production of 1 kg DINP (for GWP, ODP, AP, POCP, and EP using the CML method (CML 2001 – April 2013 (Version 4.2), see http://www.gabi-software.com/support/gabi/gabi-lciadocumentation)).

#### **Input Parameters**

Indicator	Unit	Value
		DINP
Non-renewable energy re- sources <sup>1)</sup>	MJ	78
• Fuel energy	MJ	ca. 38
Feedstock energy	мј	ca. 40
Renewable energy resources (biomass):)	MJ	0.79
Fuel energy	MJ	0.79
Feedstock energy	MJ	-
Abiotic Depletion Potential		
Elements	kg Sb eq	6.8E-07
• Fossil fuels	MJ	70
Renewable materials (bio- mass)	kg	_
Water use (key foreground pro- cess level)	kg	
for process	kg	4.5E-03
<ul> <li>for cooling</li> </ul>	kg	8.8
<sup>1)</sup> Calculated as upper heating val	ue (UHV)	

#### **Output Parameters**

Indicator	Unit	Value		
		DINP		
Global Warming Potential (GWP)	kg CO₂ eq	2.2		
Ozone Depletion Potential (ODP)	g CFC-11 eq	2.2E-07		
Acidification Potential (AP)	g SO₂ eq	5.0		
Photochemical Ozone Creation Po- tential (POCP)	g Ethene eq	1.3		
Eutrophication Potential (EP)	g PO <sub>4</sub> eq	0.39		
Dust/particulate matter <sup>2)</sup>	g PM10	0.10		
Total particulate matter <sup>2)</sup>	g	0.15		
Waste <sup>3)</sup>				
Hazardous waste	kg	4.5E-03		
Non-hazardous waste	kg	0.0		
<sup>2)</sup> Including secondary PM10				
<sup>3)</sup> From the key foreground process				

## Additional Environmental and Health Information

DINP is safe for use in all current applications. Restrictions apply for toys and childcare articles that can be placed in the mouth according to Regulation (EC) No 1907/2006, Annex XVII-52 (ECHA 2013).

## Additional Technical Information

The main properties of DINP are low volatility and density. DINP displays good resistance to aging as well as easy plastisol coating, spraying and dipping. Further, it is also compatible with secondary plasticizers.

## Additional Economic Information

Low volatility and density enables reduced process emissions and improved working conditions. The resistance to aging increases the PVC product life.

## Information

#### Data Owner

## ECPI - European Council for Plasticisers and Intermediates Cefic AISBL (The European Chemical Industry Council) Avenue E van Nieuwenhuyse 4, Box 2 B-1160 Brussels Belgium Tel.: +32 (2) 676 72 60, Fax: +32 (2) 676 73 92 E-mail: info@ecpi.org

#### **Programme Manager**

#### **DEKRA Consulting GmbH**

Registration number: PlasticsEurope 2015-004, validation expires on 30 December 2017 (date of next revalidation review).

#### LCA Practitioner and Dataset Developer

#### **PE INTERNATIONAL**

Hauptstr. 111-113 D-70771 Leinfelden-Echterdingen Germany Tel.: +49 (0)711 341 817 0, Fax: +49 (0)711 341 817 25 E-mail: consulting@pe-international.com.

#### Reviewer

#### denkstatt GmbH

This Environmental Product Declaration has been reviewed by denkstatt GmbH. It was approved according to the Product Category Rules PCR version 2.0 (2011-04) and ISO 14025:2006.

#### **Programme Owner**

#### PlasticsEurope

Avenue E van Nieuwenhuyse 4, Box 3 B-1160 Brussels Belgium Tel.: +32 (2) 675 32 97, Fax: +32 (2) 675 39 35 E-mail: info@plasticseurope.org.

For copies of this EPD, for the underlying LCI data (Eco-profile); and for additional information, please refer to <u>http://www.plasticseurope.org/</u>.

#### References

PlasticsEurope: Eco-profiles and environmental declarations – LCI methodology and PCR for uncompounded polymer resins and reactive polymer precursors (version 2.0, April 2011).



## Goal & Scope

## Intended Use & Target Audience

Eco-profiles (LCIs) and EPDs from this programme are intended to be used as »cradle-to-gate« building blocks of life cycle assessment (LCA) studies of defined applications or products. LCA studies considering the full life cycle (»cradle-to-grave«) of an application or product allow for comparative assertions to be derived. It is essential to note that comparisons cannot be made at the level of the polymer or its precursors. In order to compare the performance of different materials, the whole life cycle and the effects of relevant life cycle parameters must be considered.

PlasticsEurope Eco-profiles and EPDs represent polymer production systems with a defined output. They can be used as modular building blocks in LCA studies. However, these integrated industrial systems cannot be disaggregated further into single unit processes, because this would neglect the interdependence of the elements, e.g. the internal recycling of feedstocks and precursors between different parts of the integrated production sites.

PlasticsEurope Eco-profiles and EPDs are prepared in accordance with the stringent ISO 14040–44 requirements. Since the system boundary is »cradle-to-gate«, however, their respective reference flows are disparate, namely referring to a broad variety of polymers and precursors. This implies that, in accordance with ISO 14040–44, a direct comparison of Eco-profiles is impossible (1 kg is a declared unit, not a functional unit). While ISO 14025, Clause 5.2.2 does allow EPDs to be used in comparison, PlasticsEurope EPDs are derived from Eco-profiles, i.e. with the same »cradle-to-gate« system boundaries.

# As a consequence, a direct comparison of Eco-profiles or EPDs makes no sense because 1 kg of different polymer (additives) are not functionally equivalent.

Once a full life cycle model for a defined polymer application among several functionally equivalent systems is established, and only then, can comparative assertions be derived. The same goes for EPDs, for instance, of building product where PlasticsEurope EPDs can serve as building blocks.

Eco-profiles and EPDs are intended for use by the following target audiences:

- member companies, to support product-orientated environmental management and continuous improvement of production processes (benchmarking);
- downstream users of plastics, as a building block of life cycle assessment (LCA) studies of plastics applications and products; and
- other interested parties, as a source of life cycle information.

### **Product Category and Declared Unit**

#### **Product Category**

The core product category is defined as **uncompounded polymer resins and reactive polymer precursors**. This product category is defined »at gate« of the polymer or precursor production and is thus fully within the scope of PlasticsEurope as a federation. In some cases, it may be necessary to include one or several additives in the Eco-

profile to represent the polymer or precursor »at gate«. For instance, some polymers may require a heat stabiliser, or a reactive precursor may require a flame retardant. This special case is distinguished from a subsequent compounding step conducted by a third-party downstream user (outside PlasticsEurope's core scope).

#### Functional Unit and Declared Unit

The default Functional Unit and Declared Unit of PlasticsEurope Eco-profiles and EPDs are (unless otherwise specified<sup>1</sup>):

1 kg of primary Di-isononyl phthalate (DINP), »at gate« (DINP production site output), representing a European industry production average.

## **Product and Producer Description**

#### **Product Description**

Di-isononyl phthalate (DINP) is a phthalate used as a plasticizer in e.g. many technical products. It exists in two forms (and two CAS numbers), reflecting the two possible routes for isononanol precursor production. However their properties are similar.

Di-isononyl phthalate (DINP)

CAS no. 28553-12-0 (from C9 alcohol fraction which is n-butene based) or 68515-48-0 (from C8-10 alcohol fraction, C9-rich manufactured by the "Polygas" process).

Chemical formula  $C_{26}H_{42}O_4$  (average)

Molecular mass 418.6 g/mol (average)

Gross calorific value 36.0 MJ/kg, net calorific value 33.8 MJ/kg

DINP is used as a general, all-purpose plasticizer, 95% of which is used in PVC applications such as wire and cables, flooring, truck tarpaulins, wall covering, self-adhesive films or labels, synthetic leather, coated fabrics, technical foils, roofing membranes and automotive applications. More than half of the DINP used in non-PVC applications involves polymer related-uses (e.g. rubbers). The remaining DINP is used in inks and pigments, adhesives, sealants, paints and lacquers and lubricants (ECPI 2014).

#### **Production Process Description**

DINP is produced by esterification of phthalic anhydride with isononyl alcohol (= isononanol) in a closed system. The reaction rate is accelerated by elevated temperatures (140-250 °C) and a catalyst. Following virtually complete esterification, excess alcohol is removed under reduced pressure and the product is then typically neutralised, water washed and filtered.

#### **Producer Description**

PlasticsEurope Eco-profiles and EPDs represent European industry averages within the scope of PlasticsEurope as the issuing trade federation. Hence they are not attributed to any single producer, but rather to the European

<sup>1</sup> Exceptions can occur when reporting Eco-profiles of, for instance, process energy, such as on-site steam, or conversion processes, such as extrusion.

plasticizer industry as represented by ECPI membership and the production sites participating in the Eco-profile data collection. The following companies contributed data to this Eco-profile and EPD:

BASF SE

D- 67056 Ludwigshafen Germany <u>http://www.basf.com</u>

• Evonik Industries AG

Paul-Baumann-Straße 1 D-45772 Marl Germany http://www.evonik.com/

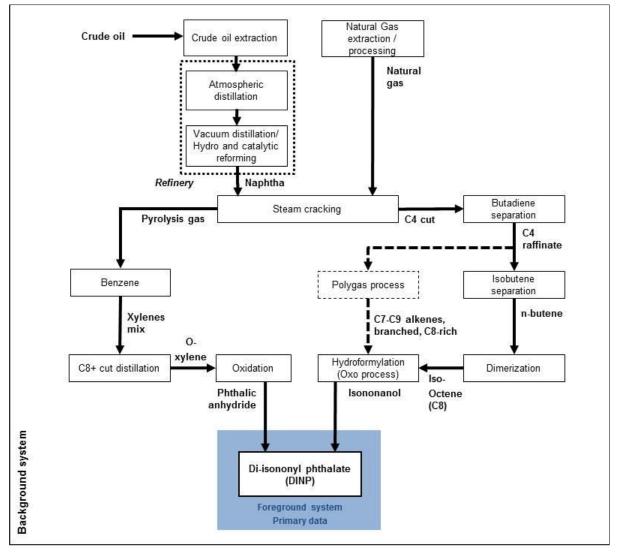
ExxonMobil Chemical Holland BV

Botlekweg 121 NL-3197 KA Rotterdam-Botlek Havennummer 4060 The Netherlands http://www.exxonmobilchemical.com/

## Eco-profile – Life Cycle Inventory

## **System Boundaries**

PlasticsEurope Eco-profiles and EPDs refer to the production of polymers and additives as a cradle-to-gate system (see Figure 1 for DINP; as far as the two isononanol precursors are concerned, the flows for C7-C9, C8-rich alkenes production by polygas process are dotted, whereas those for isooctene production by n-butene dimerization are solid).



*Figure 1: Cradle-to-gate system boundaries (DINP)* 

#### **Technological Reference**

The production processes were modelled using specific values from primary data collection at site. The main data source was a primary data collection from European producers of DINP, providing site-specific gate-to-gate production data for processes under operational control of the participating companies: three DINP producers with three plants in two different European countries. This covers 90% of the European DINP production capacity (EU-27) in 2011. Primary data were used for all foreground processes (under operational control) complemented with secondary data for background processes (under indirect management control). The data for the upstream

supply chain until the precursors are modelled from literature sources or taken from the database of the software system GaBi 6 [GABI 6 2013]. One company delivered additional primary data for the production of isononanol.

As shown in Figure 1, two different routes for the production of isononanol are modelled as per the actual supply situation (two technologies to produce the C8 alkene precursor: n-butene dimerization and polygas process). The n-butene dimerization process is based on the catalytic dimerization of n-butene and renders pure iso-octene (C8 alkene, 1- or 2-branched) as its main product. The polygas process involves the oligomerization of a C4 alkene cut: in this case, branched octenes (C8 alkenes) are the main product, with heptenes (C7 alkenes) and nonenes (C9 alkenes) as co-products. The use of one or the other technology is modelled according to site-specific information. Both octenes are then hydroformylated to yield isononanol.

#### **Temporal Reference**

The LCI data for production was collected as 12 month averages representing the year 2011, to compensate seasonal influence of data. Background data have reference years between 2010 (for electricity and thermal energy processes) and 2012. The dataset is considered to be valid until substantial technological changes in the production chain occur. In view of the latest technology development, the overall reference year for this Eco-profile is 2011, with a maximum temporal validity until 2019 for the foreground system.

#### **Geographical Reference**

Primary production data for DINP production are from three different European suppliers. Whenever applicable (in the majority of the cases), site specific conditions are applied. Only in cases where no further information is available, average European conditions are used for fuel and energy inputs in the system. Therefore, the study results are intended to be applicable within EU boundaries: adjustments might be required if the results are applied to other regions. DINP imported into Europe is not considered in this Eco-profile.

### **Cut-off Rules**

In the foreground processes all relevant flows are considered, trying to avoid any cut-off of material and energy flows. According to the GaBi database 2013 [GABI 6 2013] used in the background processes, at least 95 % of mass and energy of the input and output flows are covered and 98 % of their environmental relevance (according to expert judgment) is considered, hence an influence of cut-offs less than 2% on the total is expected (single contributions account for not more than 1%, in sum maximum 2%). Transport processes are included for the relevant material flows.

### **Data Quality Requirements**

#### **Data Sources**

Eco-profile and EPDs developed by PlasticsEurope use average data representative of the respective foreground production process, both in terms of technology and market share. The primary data are derived from site specific information for processes under operational control supplied by the participating member companies of ECPI (see Producer Description). With regard to one important intermediate, isooctene (precursor for isononanol), the participating member companies validated the datasets and their quality.

- The polygas process is based on the oligomerization of a C4 alkene cut (known as C4 raffinate): in this case, branched octenes are the main product, with heptenes and nonenes as co-products. This dataset is modelled based on literature and PE INTERNATIONAL's engineering know-how. It is cross-checked with other references and reviewed by industry representatives for plausibility and quality.
- The butene dimerization process involves the catalytic dimerization of n-butene and renders pure isooctenes (1- or 2-branched) as its main product. For one of the two producers using this route, this dataset is modelled based on literature and PE INTERNATIONALS's engineering know-how. It is cross-checked with other references and reviewed by industry representatives for plausibility and quality. The other producer provided primary data.

The data for the upstream supply chain as well as relevant background data such as energy generation and auxiliary materials are sourced from the life cycle database of the software system GaBi 6 [GABI 6 2013]. Most of the background datasets used are publicly available and documented.

#### Relevance

With regard to the goal and scope of this Eco-profile, the collected primary data of foreground processes are of high relevance, i.e. data are sourced from the most important DINP producers in Europe in order to generate a European production average. The environmental contributions of each process to the overall LCI results are included in the Chapter 'Life Cycle Impact Assessment'.

#### Representativeness

The participating companies represent 90% of the European DINP production volume in 2011. The selected background data can be regarded as representative for the intended purpose.

#### Consistency

To ensure consistency, only primary data of the same level of detail and background data from the GaBi 6 databases [GABI 6 2013] are used. While building up the model, cross-checks ensure the plausibility of mass and energy flows. The methodological framework is consistent throughout the whole model as the same methodological principles are used both in foreground and background system. In addition to the external review, an internal independent quality check was performed (see 'Internal Independent Quality Assurance Statement')

#### **Reliability & Uncertainty**

Data of foreground processes provided directly by producers were predominantly measured. Data of relevant background processes were measured at several sites – alternatively, it was determined from literature data, or estimated for some flows, which usually have been reviewed and quality checked.

The uncertainty of the background processes for the GaBi databases is described in the GaBi Database & Modelling Principles (GABI MODELLING PRINCIPLES), where also the Data Quality Indicators are described, which can be found in the documentation of the processes. A common rule estimates the best achievable uncertainty in LCA to be around 10%. Uncertainty in LCA is usually related to measurement error-determination of the relevant data, e.g. consumption or emission figures.

#### Completeness

Primary data used for the gate-to-gate production of DINP covers all related flows in accordance with the above cut-off criteria. In this way all relevant flows are quantified and data is considered complete. The elementary flows covered in the model enable the impact assessment of all selected impact categories. Waste treatment is included in the model, so that only elementary flows cross the system boundaries.

#### **Precision and Accuracy**

As the relevant foreground data are primary data, or modelled based on primary information sources of the owners of the technologies, precision is deemed appropriate to the goal and scope.

#### Reproducibility

Reproducibility is given for internal use since the owners of the technologies provided the data under confidentiality agreements. Key information is documented in this report, and data and models are stored in the GaBi 6 software database. Sub-systems are modelled by ´state of art´ technology using data from a publicly available and internationally used database. It is worth noting that for external audiences, full and detailed reproducibility will not be possible for confidentiality reasons. However, experienced practitioners could reproduce suitable parts of the system as well as key indicators in a certain confidence range.

#### **Data Validation**

The data on production collected from the project partners and the data providing companies was validated in an iterative process several times. The collected data was validated using existing data from published sources or expert knowledge. The background information from the GaBi database is updated regularly and continuously validated.

#### Life Cycle Model

The study has been performed with the LCA software GaBi 6 [GABI 6 2013]. The associated database integrates ISO 14040/44 requirements. Due to confidentiality reasons details on software modelling and methods used cannot be shown here. However, provided that appropriate confidentiality agreements are in place the model can be reviewed in detail; an external independent review was conducted to this aim. The calculation follows the vertical calculation methodology (see below).

#### **Calculation Rules**

#### **Vertical Averaging**

When modelling and calculating average Eco-profiles from the collected individual LCI datasets, vertical averages are calculated (Figure 2).

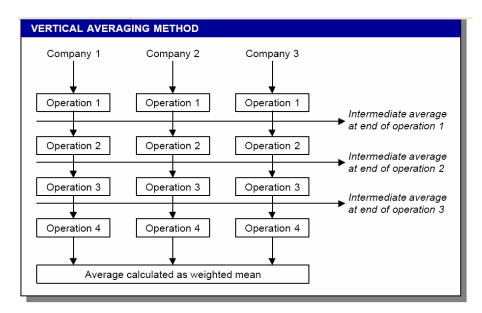


Figure 2:

*Vertical Averaging (source: Eco-profile of high volume commodity phthalate esters, ECPI European Council for Plasticisers and Intermediates, 2001)* 

#### **Allocation Rules**

Production processes in chemical and plastics industry are usually multi-functional systems, i.e. they have not one, but several valuable product and co-product outputs. Wherever possible, allocation should be avoided by expanding the system to include the additional functions related to the co-products. Often, however, avoiding allocation is not feasible in technical reality, as alternative stand-alone processes do not exist or even alternative technologies show completely different technical performance and product quality output. In such cases, the aim of allocation is to find a suitable partitioning parameter so that the inputs and outputs of the system can be assigned to the specific product sub-system under consideration.

#### Foreground system

Where co-products of DINP production are relevant, price allocation is applied, because they are marketed as well. These products have much lower assignments compared to the main product DINP. The purpose of the processes is the production of DINP. A quantified sensitivity analysis shows that if mass allocation is applied, results would differ by about 0.5% maximum in all impact categories analysed in this report. No post-consumer waste has been reported as input to the system, therefore no allocation between different life cycles is necessary.

The overall production of the participating companies comprises further products beside the product considered in this study. Data for thermal and electrical energy as well as auxiliary material refer to the declared product. During data collection the allocation is done e.g. via mass, area, pieces or time spent in the machine.

#### Background system

In the refinery operations, co-production was addressed by applying allocation based on mass and net calorific value [GABI 6 2013]. The manufacturing route of every refinery product is modelled and so the effort of the production of these products is calculated specifically. Two allocation rules are applied: 1. the raw material (crude oil) consumption of the respective stages, which is necessary for the production of a product or an intermediate product, is allocated by energy (mass of the product \* calorific value of the product); and 2. the energy consumption (thermal energy, steam, electricity) of a process, e.g. atmospheric distillation, being required by a product or an intermediate product, are charged on the product according to the share of the throughput of the stage (mass allocation).

The chosen allocation in refinery is based on several sensitivity analyses, which was reviewed by petrochemical experts. The relevance and influence of different possible allocation keys in this context is small. In steam cracking, allocation according to net calorific value with regard to the whole product range was applied. The difference compared with mass allocation is below 2%.

Materials and chemicals needed during manufacturing are modelled using the allocation rule most suitable for the respective product. For further information on a specific product see <u>documentation.gabi-software.com</u>. For the generation of life cycle inventories for electrical and thermal energy beside above mentioned allocation methods for refinery products and materials allocations by economic value are applied, dependent on the specific technique. In case of plants for the co-generation of heat and power allocations by exergy are applied.

## Life Cycle Inventory (LCI) Results

#### Formats of LCI Dataset

The Eco-profile is provided in four electronic formats:

- As input/output table in Excel<sup>®</sup>
- As XML document in EcoSpold format (<u>www.ecoinvent.org</u>)
- As XML document in ILCD format (<u>http://eplca.jrc.ec.europa.eu/</u>)
- As GBX file in GaBi format (www.gabi-software.com)

Key results are summarised below.

#### **Energy Demand**

As a key indicator on the inventory level, the **primary energy demand** (system input) of 78.84 MJ/kg DINP indicates the cumulative energy requirements at the resource level, accrued along the entire process chain (system boundaries), quantified as gross calorific value (upper heating value, UHV).

As a measure of the share of primary energy incorporated in the product, and hence indicating a recovery potential, the **energy content in the plasticizer** (system output), quantified as the gross calorific value (UHV), is 36.0 MJ/kg for DINP. The net calorific value (lower heating value, LHV) is 33.6 MJ/kg DINP.

Table 1:	Primary energy demand (system boundary level) per 1kg DINP
Tubic 1.	Thinking chergy demand (System boundary level) per 1kg binn

Primary Energy Demand	Value [MJ]
Energy content in polymer (energy recovery potential, quantified as gross calorific value of plasti-	36
cizer)	
Process energy (quantified as difference between primary energy demand and energy content of	43
polymer)	
Total primary energy demand	79

Consequently, the difference ( $\Delta$ ) between primary energy input and energy content in plasticizer output is a measure of **process energy** which may be either dissipated as waste heat or recovered for use within the system boundaries. Useful energy flows leaving the system boundaries were removed during system expansion.

Table 2 shows how the total energy input (primary energy demand) is used as fuel or feedstock. Fuel use means generating process energy, whereas feedstock use means incorporating hydrocarbon resources into the plasticizer. Note that some feedstock input may still be valorised as energy; furthermore, process energy requirements may also be affected by exothermic or endothermic reactions of intermediate products. Hence, there is a difference between the feedstock energy input and the energy content of the plasticizer (measurable as its gross calorific value). Considering this uncertainty of the exact division of the process energy as originating from either fuels or feedstocks, as well as the use of average data (secondary data) in the modelling with different country-specific grades of crude oil and natural gas, the feedstock energy is presented as approximate data.

Primary energy re-	Total Energy Input	Total Mass Input [kg]	Feedstock Energy In-	Fuel Energy Input
source input	[MJ]		put [MJ]	[MJ]
Coal	2.1	0.077	0.0	2.1
Oil	37	0.82	ca. 20	ca. 17
Natural gas	37	0.75	ca. 20	ca. 17
Lignite	0.93	0.069	0.0	0.93
Nuclear	1.0	2.3E-06	0.0	1.0
Biomass	0.0	0.0	0.0	0.0
Hydro	0.14	-	0.0	0.14
Solar	0.43	-	0.0	0.43
Geothermics	2.2E-03	-	0.0	2.2E-03
Waves	2.2E-13	-	0.0	2.2E-13
Wood	0.0	0.0	0.0	0.0
Wind	0.22	-	0.0	0.22
Other renewable				
fuels	0.0	-	0.0	0.0
Sub-total renewable	0.79	0.0	0.0	0.79
Sub-total Non-renew-	-0			
able	78	1.7	ca. 40	ca. 38
Total	79	1.7	ca. 40	ca. 39

Table 2:Analysis by primary energy resources (system boundary level), expressed as energy and/or mass<br/>(as applicable) per 1 kg DINP

Table 3 shows that nearly all of the primary energy demand is from non-renewable resources.

Since the focus scope of ECPI and its member companies is plasticizer production, Table 4 analyses the types of useful energy inputs in the DINP production process: Electricity has a minor contribution here, whereas the majority is thermal energy (heat). This represents the share of the energy requirement that is under operational control of the polymer producer (Figure 3). Accordingly, Table 5 shows that the majority (99%) of the primary energy demand is accounted for by upstream processes. Finally, Table 6 provides a more detailed overview of the key processes along the production system, their contribution to primary energy demand and how this is sourced from the respective energy resources. This puts the predominant contribution of the production into perspective with the precursors (»other chemicals«). It should be noted, however, that the LCI tables in the annex account for the entire cradle-to-gate primary energy demand of the DINP system.

Table 3:

#### Primary energy demand by renewability per 1 kg DINP

Fuel/energy input type	Value [MJ]	%
Renewable energy resources	0.79	1%
Non-renewable energy resources	78	99%
Total	79	100%

Table 4:

Analysis by type of useful energy (DINP production – unit process level) per 1 kg DINP

Type of useful energy in process input	Value [MJ]
Electricity	8.1E-02
Heat, thermal energy	1.3
Other types of useful energy (relevant contributions to be specified)	0.0
Total (for selected key process)	1.4

Table 5:

Contribution to primary energy demand (dominance analysis) per 1 kg DINP

Contribution to Primary Energy per segment	Value [MJ]	%
DINP Production (electricity, steam, unit process, utilities, waste treat- ment)	1.3	2%
Pre-chain	77.5	98%
Total	79	100%

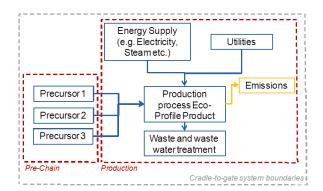
#### Table 6:

*Contribution of life cycle stages to total primary energy demand (gross calorific values) per 1 kg DINP, see Figure 3* 

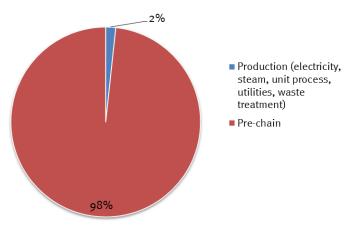
Total Primary Energy [MJ]	DINP precursors and process*	Other Chemicals	Utilities	Electricity	Thermal Energy	Transport	Process Waste Treatment
Coal	1.8	6.4E-03	4.2E-02	6.3E-02	0.20	7.4E-05	-1.1E-02
Oil	37	0.43	9.0E-03	2.6E-03	7.8E-03	1.5E-02	-7.7E-02
Natural gas	36	0.26	2.9E-02	0.12	0.91	1.2E-03	-1.4E-02
Lignite	0.91	6.2E-03	4.4E-03	6.9E-03	2.7E-03	1.9E-05	-1.3E-04
Nuclear	1.0	6.9E-03	6.0E-03	3.6E-03	2.7E-03	3.9E-05	-3.5E-04
Biomass							
Hydro	0.14	9.9E-04	1.1E-03	3.1E-04	4.8E-04	1.0E-05	-7.6E-05
Solar	0.41	2.4E-03	1.5E-03	1.2E-02	1.1E-03	4.6E-04	-3.2E-03
Geothermics	2.1E-03	1.7E-05	4.4E-05	3.3E-06	3.4E-06	3.2E-07	-1.8E-06
Waves	2.2E-13	1.9E-15	7.2E-16	2.3E-16	6.5E-16	2.5E-18	-6.5E-17
Wood							
Wind	0.21	1.4E-03	1.0E-03	9.2E-04	5.7E-04	8.1E-06	-1.0E-04
Other renewa- ble fuels			-				·
Total	77	0.71	9.4E-02	0.21	1.1	1.7E-02	-0.11

\* Precursors and process include phthalic anhydride, isononanol and direct process emissions.

\*\* Utilities include e.g. inert gases, compressed air, water, filter media as well as catalyst



## **Contribution to Primary Energy Demand**



*Figure 3: Contribution to primary energy demand per segment* 

#### Water Use and Consumption

Table 7 shows the water use at cradle-to-gate level. Water use (incl. fresh-, rain- and seawater; also categorized as blue- and green water) equals the measured water input into a product system or process. Blue water refers to surface and groundwater, green water to rain water. Water use is the total amount of water withdrawn from its source (water abstraction). The term "water consumption" refers to the amount of water removed from, but not returned to, the same drainage basin [ISO 14046: 2014].

Input	Value [kg
Water (ground water)	13
Water (lake water)	17
Water (rain water)	1.3
Water (river water)	6.3E+02
Water (sea water)	2.0
Water (fossil groundwater)	0.0

Table 8 provides the corresponding freshwater part in the water balance. Freshwater is naturally occurring water on the Earth's surface in ponds, lakes, rivers and streams, as ice, and underground as groundwater in aquifers and underground streams. The term specifically excludes seawater and brackish water.

Input	Value [kg]
Water (ground water)	13
Water (lake water)	17
Water (river water)	6.3E+02
Water (fossil groundwater)	0.0
Total fresh water use [kg]	6.7E+02
Output	Value [kg]
Water (river water from technosphere, cooling water)	26
Water (river water from technosphere, turbined)	6.2E+02
Water (river water from technosphere, waste water)	4.7
Water (lake water from technosphere, cooling water)	0.0
Water (lake water from technosphere, turbined)	0.0
Water (lake water from technosphere, waste water)	0.0
Total fresh water release from technosphere (degradative use) [kg]	6.5E+02

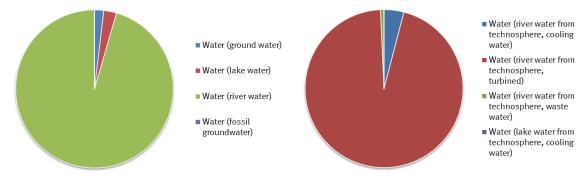


Figure 4:

Total fresh water use and release (DINP)

Table 9 shows the water balance at unit process level.

Water balance table per 1 kg DINP (water use and release at unit process level)

Input	Value [kg
Water (cooling water)	8.8
Water (process water)	4.4E-03
Water (deionised)	0.14
Water (ground water)	0.0
Output	Value [kg
Water vapour	0.34
Water (waste water, untreated) to waste water treatment plant (WWTP)	0.15
Water direct released to the environment without WW	<u>TP</u>
Water (river water from technosphere, cooling water)	8.5
Water (river water from technosphere, turbined)	0.0
Water (river water from technosphere, waste water)	0.0
Water (sea water from technosphere, cooling water)	0.0
Water (sea water from technosphere, turbined)	0.0
Water (sea water from technosphere, waste water)	0.0
Water (lake water from technosphere, cooling water)	0.0
Water (lake water from technosphere, turbined)	0.0

#### **Air Emission Data**

Table 10 shows a few selected air emissions which are commonly reported and used as key performance indicators; for a full inventory of air emissions, please refer to the complete LCI table in the annex of this report.

Table 10:	Selected air emissions per 1 kg DINP

Air emissions	kg
Carbon dioxide, fossil (CO₂, fossil)	1.9
Carbon monoxide (CO)	1.4E-03
Methane (CH <sub>4</sub> )	8.oE-o3
Sulphur dioxide (SO₂)	3.0E-03
Nitrogen oxides (NOx)	2.3E-03
Particulate matter ≤ 10 µm (PM 10)	1.0E-04

#### **Wastewater Emissions**

Table 11 shows a few selected wastewater emissions which are commonly reported and used as key performance indicators; for a full inventory of wastewater emissions, please refer to the complete LCI table in the annex of this report.

Table 11:Selected water emissions per 1 kg DINP

Water emissions	kg
Biological oxygen demand after 5 days (BOD 5)	2.8E-05
Chemical oxygen demand (COD)	5.7E-04
Total organic carbon (TOC)	2.0E-05

### Solid Waste

Table 12 below lists the solid wastes before treatment.

Waste for –	Incineration	Landfill	Recovery	Unspecified	Total
	kg	kg	kg	kg	kg
Non-hazardous	0.0	0.0	0.0	0.0	0.0
Hazardous	2.2E-03	0.0	2.3E-03	0.0	4.5E-03
Unspecified	0.0	0.0	0.0	0.0	0.0
Total	2.2E-03	0.0	2.3E-03	0.0	4.5E-03

 Table 12:
 Solid waste generation per 1 kg DINP (key foreground process level)

## Life Cycle Impact Assessment (LCIA)

For the calculation of the LCIA the CML methods (CML 2001 – April 2013 (Version 4.2), see <u>http://www.gabi-soft-ware.com/support/gabi/gabi-lcia-documentation</u>) were used.

#### Input

#### **Natural Resources**

Table 13 shows the potential depletion of non-living natural resources extracted from earth caused by the production of 1 kg DINP. It is measured by two impact categories: Abiotic Depletion Potential for elements expressed in Antimony (Sb) equivalents and Abiotic Depletion Potential for fossil fuels expressed in MJ.

Table 13:	Abiotic Depletion Potential per 1 kg DINP

Natural resources	Value
Abiotic Depletion Potential (ADP), elements [kg Sb eq]	6.8E-07
Abiotic Depletion Potential (ADP), fossil fuels [MJ]	71

### Output

#### **Climate Change**

In table 14 the influence on climate change of the greenhouse gases emitted along the DINP production chain is displayed. It is expressed as Global Warming Potential (100 years) in kg carbon dioxide equivalents.

 Table 14:
 Global Warming Potential (100 years) per 1 kg DINP

Climate change	kg CO₂ eq.
Global Warming Potential (GWP)	2.2

#### Acidification

Table 15 shows the potential acidification caused by the production of DINP, via the emissions of acid gases (such as  $SO_2$  or NO<sub>2</sub>) into the air. It is expressed as Acidification Potential in g sulphur dioxide equivalents.

Table 15:Acidification Potential per 1 kg DINP

Acidification of soils and water bodies	g SO₂ eq.
Acidification Potential (AP)	5.0

#### Eutrophication

Table 16 displays the potential eutrophication mainly due to phosphor- and nitrogen-containing compounds emitted in water, soil and air along the DINP production chain. It is expressed as Eutrophication Potential in g phosphate equivalents.

Table 16:

Eutrophication Potential per 1 kg DINP

Eutrophication of soils and water bodies	g PO₄³ <sup>.</sup> eq.
Eutrophication Potential (EP), total	0.39

#### **Ozone Depletion**

Halogenated emissions to air such as CFCs (chlorofluorocarbons) contribute to reduce the stratospheric ozone layer. This effect is displayed in Table 17 as Ozone Depletion Potential, expressed in g CFC-11 equivalents per 1 kg DINP.

Table 17:

Ozone Depletion Potential per 1 kg DINP

	g CFC-11 eq.
Ozone Depletion Potential (ODP)	2.2E-07

#### Summer Smog

Summer smog is formed when heat from the sun causes ozone to build up in the troposphere, upon combination of nitrogen oxides and volatile organic compounds (VOCs) emitted in air. This effect is assessed in Table 18 as Photochemical Ozone Creation Potential, in g ethene equivalents per 1 kg DINP.

 Table 18:
 Photochemical Ozone Creation Potential per 1 kg DINP

	g Ethene eq.
Photochemical Ozone Creation Potential (POCP)	1.3

#### **Dust & Particulate Matter**

Fuel combustion processes occurring in vehicles, power plants and some industrial processes are sources of emissions of particulate matter (PM) suspended in the Earth's atmosphere. Table 19 lists the emissions of particles under 10 µm, split between direct PM emissions, or PM formed from the oxidation of primary gases, expressed in g PM 10 equivalents.

Table 19:PM10 emissions per 1 kg DINP

Particulate matter	g PM10 eq.
Particulate matter $\leq$ 10 $\mu$ m. total	0.10
Particulate matter $\leq$ 10 $\mu m$ (direct emissions)	0.0
Particulate matter $\leq$ 10 $\mu m$ (secondary)	0.10

Considering the PM > 10  $\mu$ m amounting to 4.7E-02 g, the total particulate matter emissions are 0.15 g per 1 kg DINP

#### **Dominance Analysis**

Table 20 shows the main contributions to the results presented above. A weighted average of the different technologies represented by the participating producers is used. Regarding DINP, in all analysed environmental impact categories, intermediates contribute with about 94% or more of the total impact, with INA and phthalic anhydride dominating all cases. The negative POCP impact due to transport is caused by nitrogen monoxide emissions that contribute to reduce tropospheric ozone. Moreover, the negative impact results reported for process waste treatment in 4 impact categories are due to the energy recovery upon waste incineration and therefore the energy credit given for the recovered energy.

	Total Primary En- ergy [MJ]	ADP Elements [kg Sb eq.]	ADP Fossil [MJ]	GWP [kg CO₂ eq.]	AP [g SO₂ eq.]	EP [g PO₄ <sup>3•</sup> eq]	POCP [g Ethene eq.]
DINP precursors and pro- cess*	97%	96%	97%	95%	96%	96%	98%
Other chemicals	0.90%	1.9%	0.91%	0.90%	0.89%	0.94%	1.4%
Utilities**	0.12%	0.65%	0.11%	0.31%	1.4%	0.35%	0.21%
Electricity	0.27%	0.29%	0.25%	0.64%	0.31%	0.48%	0.11%
Thermal Energy	1.4%	0.73%	1.45%	3.3%	1.5%	2.15%	0.62%
Transport	2.2E-02%	6.8E-05%	2.2E-02%	5.3E-02%	0.11%	0.26%	-4.9E-02%
Process waste treatment	-0.13%	5.8E-02%	-0.13%	9.2E-02%	-0.13%	8.9E-02%	-0.12%
Total	100. %	100%	100%	100%	100%	100%	100%

#### Table 20:Dominance analysis of impacts per 1kg DINP

\* Precursors and process include phthalic anhydride, isononanol and direct process emissions.

\*\* Utilities include e.g. inert gases, compressed air, water, filter media as well as catalyst

#### Comparison of the Present Eco-profile with its Previous Version (2001/2014)

In 2001, an Eco-profile of high volume commodity phthalate esters (DEHP/DINP/DIDP) was carried out [ECOBILAN 2001]. However, no detailed information on foreground data and applied background LCIs is available in the document to enable precise comparison with the current Eco-profile. Moreover, in that past Eco-profile, only LCI data was published, but no life cycle impact assessment results such as reported here.

For these reasons, a quantitative comparison of the results of both Eco-profiles is not really relevant; instead, below are listed the various changes identified between the two Eco-profile versions which can provide a qualitative explanation of the differences:

• Changes in scope:

The 2001 Eco-profile was aggregating and averaging assessments for three phthalate plasticizers (DEHP, DINP and DIDP), instead of only DINP in the current document. As shown in <a href="http://www.plasticisers.org/en\_GB/plasticisers/high-phthalates">http://www.plasticisers.org/en\_GB/plasticisers/high-phthalates</a>, at the time of the previous study, the high phthalate esters production was largely dominated by DEHP, whereas DINP was in minority. Ethylhexyl alcohol, the main precursor for DEHP, is produced by aldolization of butyraldehyde made from propene and syngas, a technology quite different from the oligomerization of olefins and hydroformylation route for the DIDP and DINP precursor alcohols.

• Changes in data sources:

The 2001 Eco-profile was based on site-specific data not only for the esterification process, but also all intermediates manufacturing (C8-C9 olefins, C9-C10 alcohols, syngas). In the current document, literature-based data and expert knowledge are used to model the precursor production, except for one manufacturer that provided site-specific primary data.

- Changes in the foreground system:
  - Energy use has been continuously improved within the plasticizer plants as well as precursor production facilities, for instance through better energy integration within the processes. This may result in an overall reduced primary energy demand and global warming potential.
  - Stricter waste, pollution and emissions control, such as exhaust air purification and waste management throughout the supply chain and the plasticizer production itself could possibly lead to decreased values in AP and EP categories.
- Changes in the background system: Changes in the electricity grid mix, in particular electricity from renewables becoming relevant, can have caused changes in all impact categories.
- Methodological changes:

Compared with the 2001 version, the system boundaries now include the waste treatment of all wastes occurring in the process, so that only elementary flows cross the system boundary: this can cause small changes in all impact categories. Please note that for the sake of comparability, waste arising is also reported on a foreground unit process level.

## **Reviews**

## Internal Independent Quality Assurance Statement

As part of the overall quality assurance during the preparation of this Eco-profile, *PE INTERNATIONAL AG* conducted an internal review of this work. The resulting quality assurance statement is reproduced in the Internal Independent Quality Assurance Statement:

On behalf of PE INTERNATIONAL AG and its subsidiaries

Document prepared by	Anja Lehmann
Title	Project Manager
Signature	A. Lehmann
Date	
Quality assurance by	Angela Schindler

Title

Signature

Angela Schadlo

Quality Manager Central Europe

Date

Approved by

Title

Signature

Hannes Partl Regional Director Central Europe, Service

Date

This report has been prepared by PE INTERNATIONAL with all reasonable skill and diligence within the terms and conditions of the contract between PE and the client. PE is not accountable to the client, or any others, with respect to any matters outside the scope agreed upon for this project.

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## **External Independent Review Summary**

#### **Review Summary**

The European Council for Plasticisers and Intermediates (ECPI), sector group of The European Chemical Industry Council (CEFIC), commissioned PE International to conduct an LCA study with the goal to setup a PlasticsEurope Eco-profile and Environmental Product Declaration (EPD) of the **plasticiser Di-isononyl phthalate (DINP)**. This critical review of the study was performed by denkstatt GmbH.

The main task of this project was to carry out a life cycle assessment (LCA) to analyse the environmental aspects which are associated with DINP. The Functional Unit of this PlasticsEurope Eco-profile and EPD is: 1 kg of primary Di-isononyl phthalate (DINP), wat gate« (DINP production site output), representing a European industry production average.

The critical review of the LCA study was established between July 2014 and January 2015. It did not involve a review of the calculations made in the study so that the findings are based on the draft (final) eco-profile report, spot-checks of the model and intensive communication with the study authors. Questions and recommendations were discussed and the report was adapted accordingly.

The LCA should be consistent with the Eco-profiles Methodology, Product Category Rules (PCR) and Protocol as given in the PlasticsEurope Eco-profile and EPD methodology document for Uncompounded Polymer Resins and Reactive Polymer Precursors [PLASTICSEUROPE 2011]. Furthermore the Eco-profile and EPD document should be in accordance with [ISO 14025: 2006], where basic principles and procedures to establish Type-III environmental declarations are standardised.

As a consequence, the critical review statement is based on the main guiding principles defined in the international standard series [ISO 14040: 2006] and []. The aim of the review was to examine that:

- methods used are scientifically and technically valid for the given goal and scope of the study;
- data used are appropriate, sufficient and reasonable in respect to the goal and scope of the study;
- conclusions drawn reflect the goal and scope of the study and the limitations identified;
- report is transparent and consistent.

In accordance with the above mentioned guiding principles the following conclusions can be drawn from the review process:

- The widely accepted state-of-the-art methodology was adopted in this LCA study and has fulfilled all necessary steps in an adequate and highly sufficient manner within the given goal of the study. Thus the study is scientifically and technically adequate.
- Quality of required data and data sources as well as data collection procedures are appropriate, sufficient and reasonable. They are in accordance with the goal and scope of the study.
- The report has been established in a clear, transparent and consistent way.
- Three European DINP producers covering 90% of the European production capacity (EU27) delivered sitespecific data for processes under their operational control. The upstream supply chain up to the precursors was modelled based on data from literature as well as GaBi 6 database. One producer additionally supplied primary data for a specific precursor.
- For the foreground system price allocation was applied where co-products of DINP production were relevant, while for the background system both energy and mass allocations were applied. Sensitivity analyses showed that the influence of different allocation keys on the results is small.
- Potential environmental impacts are dominated by precursors and direct process emissions. In total other processes contribute with 5% or less to the potential impacts.

- A comparison with the previous Eco-profile conducted by Ecobilan [ECOBILAN 2001] was made. In the current Eco-profile, only one plasticiser was used, whereas in the previous eco-profile three high volume commodity phthalate esters including Di-2-ethylhexyl phthalate (DEHP) and Di-isodecyl phthalate (DIDP) as well as DINP were considered. In addition further changes were made (data sources, system, methodology). All differences are described in the report. Due to these differences a quantitative comparison of the results of both Eco-profiles was considered to be not reasonable and hence was not carried out.
- Framework requirements, principles and procedures for Type-III environmental declarations are fulfilled.

It can be concluded that this is a competent study, which gives a thorough picture of the potential environmental impacts of Di-isononyl phthalate from cradle (crude oil extraction) to gate (product at plant). The study complies with the requirements postulated in the PlasticsEurope Eco-profile and EPD methodology document as well as the ISO 14025. Results presented in the Eco-profile and EPD are regarded being up-to-date high quality environmental data of European DINP production.

#### Names and affiliations of reviewers:

Bernd Brandt, Senior Consultant, DI, denkstatt GmbH, Vienna, Austria

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