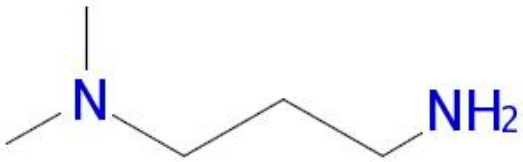
Date: 07/06/2017

Environmental Fact Sheets (#26)

Dimethylaminopropylamine (DMAPA)

petrochemical surfactant precursor

Substance Identification			
IUPAC Name	N,N-dimethylpropane-1,3-diamine	**CAS Number**	109-55-7
Other Names	1-Amino-3-dimethylaminopropane; 3-aminopropyldimethylamin; DMAPA		
Molecular Formula	C5H14N2	Structural formula: 	

Physical/Chemical Properties [1]	
Molecular Weight	102.18 g/mol
Physical state	Liquid
Appearance	Colourless
Odour	Like amines
Density	813.3 kg/m³ at 25°C
Melting Points	-60°C
Boiling point	135.1 °C at 1013.25 hPa
Flash Point	30-35°C at 1013.25 hPa
Vapour Pressure	6 hPa at 20 °C
Water Solubility	Miscible
Flammability	Study scientifically unjustified
Explosive Properties	No data available
Surface Tension	No data available
Octanol/water Partition coefficient (Kow)	log K_{OW} =-0.352 at 25°C
Product and Process Description	3-Dimethylaminopropylamine (DMAPA) is a surfactant precursor. 3-Dimethylaminopropylamine (DMAPA) is commercially produced via the reaction between dimethylamine and acrylonitrile to produce dimethylaminopropionitrile (DMAPN). Subsequent hydrogenation of DMAPN yields a crude reaction mixture that contains 95.2% of the desired DMAPA. After distillation a total yield of 91% pure DMAPA as well as 9% of co-products is received of which nearly 5% are recycled to further reaction in the DMAPN-production [5].
Application	DMAPA is used in cosmetics products, personal care products, shampoos, washing and dishwashing detergents, agricultural chemicals, fungicides, ion exchange resins, phthalocyanine dyes, and water-resistant textile fibres.

Life Cycle Assessment

General Introduction

These Environmental Fact Sheets are a product of the *ERASM Surfactant Life Cycle & Ecofootprinting (SLE)* project. The objective of this project was to establish or update the current environmental profile of 15 surfactants and 17 precursors, taking into consideration actual surfactant production technology and consistent high quality background data.

The Fact Sheets are based upon life cycle assessment (LCA) and have been prepared in accordance with the ISO standard [ISO 14040: 2006 and ISO 14044: 2006]. In addition, the project follows the ILCD (2010) handbook. This Fact Sheet describes the cradle-to-gate production for DMAPA. DMAPA is a petrochemical surfactant precursor.

The ERASM SLE project recommends to use the data provided in a full 'cradle-to-grave' life cycle context of the surfactant in a real application.

Further information on the ERASM SLE project and the source of these datasets can be found in [2].

The full LCI can be accessed via www.erasm.org or via http://lcdn.thinkstep.com/Node/

Goal and Scope of ERASM SLE Project [2]

The main goal was to update the existing LCI inventories [3] for the production of DMAPA.

Temporal Coverage	Data collected for production refer to literature research covering recent production technology. The reference year was set up to 2011. Background data have reference years from 2008 to 2010 for electricity and thermal energy processes. The dataset is considered to be valid until substantial technological changes in the production chain occur.
Geographical Coverage	Data for DMAPA came from internal database and covers European conditions. The geographical representativeness for DMAPA was considered 'good'.
Technological Coverage	The technological representativeness for DMAPA was considered 'good'. Figure 1 provides a schematic overview of the production process of DMAPA.
Declared Unit	In ERASM SLE project the declared unit (functional unit) and reference flow is one thousand kilogram (1000 kg) of surfactant active ingredient. This was the reference unit also used in [3]. Functional Unit: 1 metric tonne of DMAPA 100% active substance.
Cradle-to Gate System Boundaries	

Included	Excluded
3-(Dimethylamino)propionitril (DMAPN) production	Construction of major capital equipment (Infrastructure)
Butyl acrylate production	Maintenance and operation of support equipment
Titanium isopropoxide production	Human labor and employee transport
Dioctyltin oxide production	Packaging
Energy production	
Utilities	
Transportation processes for the main materials	
Water use and treatment of waste water	
Treatment of wastes	

Assumptions and Limitations	The modelling is based on secondary data from literature. The amounts of cooling water as well as for process energy are estimated by existing models for similar production technologies.
Cut-off Criteria [4]	No significant cut-offs were used. The LCI study included all material inputs that had a cumulative total (refers to unit process level) of at least 98% of the total mass inputs to the unit process, and included all material inputs that had a cumulative total of at least 98% of total energy inputs to the unit process.

	The study included any material that had environmental significance in its extraction, manufacture, use or disposal, is highly toxic, dangerous for the environment, or is classified as hazardous waste. The sum of the excluded material flows did not exceed 5% of mass, energy or environmental relevance.	
Calculation Rules	Allocation	No allocation was applied.
	Aggregated data	From public data and literature research.

Life Cycle Inventory and Impact Assessment [2]

Based on the LCI data an environmental impact assessment was performed for the indicators Primary Energy Demand (PED) and Global Warming Potential (GWP). Other impacts may be calculated from the full LCI dataset.

Table 1. Primary Energy Demand and air emissions related to Global Warming per 1 tonne of DMAPA 100% active substance

LCI result	Unit	Amount
Primary energy demand		
Primary energy demand from renewable materials (net calorific value)	MJ	1517
Primary energy demand from fossil materials (net calorific value)	MJ	106456
Primary energy demand from fossil and renewable materials (net calorific value)	MJ	107973
Air emissions related to Global Warming Potential		
Carbon uptake, biotic	kg CO_2 equiv.	-53.2
Carbon dioxide, fossil	kg	4401
Carbon dioxide, biotic	kg	94
Carbon dioxide, from land use, land use change and peat oxidation	kg	-
Methane	kg	12.91
Nitrous oxide (laughing gas)	kg	0.44
NMVOC emissions	kg	2.70
*Total GWP (according to [**IPCC 2007**])*	*t CO_2-equiv.*	*4.89*

Primary Energy Demand (PED): An analysis of the inventory data shows that the PED impact is mainly caused by the production of raw materials dimethylamine (DMA), and n,n-dimethylaminopropionitril (DMAPN). The precursors DMA and DMAPN represent the highest input by mass and contribute 32% and 58% to the total primary energy demand. The reactant hydrogen accounts 8% of the primary energy demand. The remaining contribution is due to electricity supply, generation of thermal energy, use of catalyst, direct emissions, water use, waste and waste water treatment.

Global Warming Potential (GWP): An analysis of the inventory data shows that the GWP impact is mainly caused by the production of raw materials dimethylamine (DMA), and n,n-dimethylaminopropionitril (DMAPN). The precursors DMA and DMAPN represent the highest input by mass and contribute 27% and 59% to the total impact of global warming potential. The reactant hydrogen accounts 9% of the GWP. The remaining contribution is due to electricity supply, generation of thermal energy, use of catalyst, direct emissions, water use, waste and waste water treatment.

References for the ERASM SLE Project	
Data Owner and Commissioner of the study	ERASM (Environment & Health Risk Assessment and Management). A research partnership of the Detergents and Surfactants Industries in Europe (www.erasm.org).
LCA Practitioner	thinkstep AG (www.thinkstep.com)
Reviewers	Prof. Walter Kloepffer, LCA Consult Mrs. Charlotte Petiot and Dr. Yannick Leguern, BiolS by Deloitte
References	[1] ECHA. http://echa.europa.eu [2] Schowanek. D. *et al*. (2017). New and Updated Life Cycle Inventories for Surfactants used in European Detergents: Summary of the ERASM Surfactant Life Cycle and Ecofootprinting Project. Int J. LCA, in press. [3] CEFIC-Franklin (1994). Resource and environmental profile analysis of petrochemical and oleo chemical surfactants produced in Europe. Phase II Final Report, Franklin Associates, LTD. [4] PLASTICSEUROPE (2011). Eco-profiles and Environmental Declarations – Life Cycle Inventory (LCI) Methodology and Product Category Rules (PCR) for Uncompounded Polymer Resins and Reactive Polymer Precursors, version 2.0. [5] Ernst, M.. BASF SE, Verfahren zur Synthese von N, N-Dimethyl-1,3- Diaminopran (DMAPA), EU-patent EP 1 945 603 B1.

Figure 1. Production process of DMAPA.