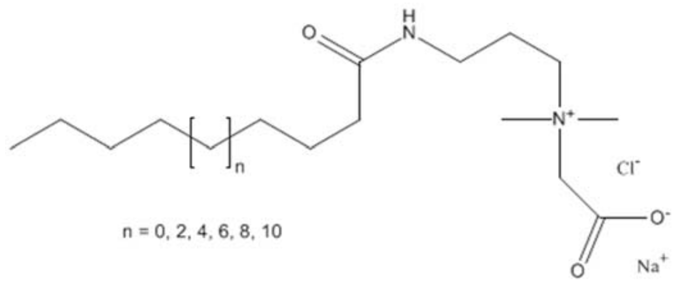
Date: 07/16/2017

Environmental Fact Sheet (#28)

C8-18 Alkyl Amidopropyl Betaine (CAPB)

oleo/petrochemical amphoteric surfactant

Substance Identification			
IUPAC Name	1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-C8-18(even numbered) acyl derivs., hydroxides, inner salts	**CAS Number**	No CAS number 931-296-8 (EC-Nr.)
Other Names	C8-18 Alkyl Amidopropyl Betaine		
Molecular Formula	UVCB substance (substances of Unknown or Variable composition, Complex reaction products or Biological materials), no univocal molecular formula available	Structural formula: 	

Physical/Chemical Properties [1]	
Molecular Weight	345.86 – 486.13
Physical state	Solid
Appearance	Powder
Odour	No data available
Density	1.15 g/cm³ at 20°C
Melting Points	Not identifiable due to decomposition in the range between 208 and 280°C
Boiling point	Not identifiable due to decomposition of the test material in the range between 208 and 280°C
Flash Point	Study scientifically unjustified (irrelevant property for solids)
Vapour Pressure	<= 0.0031 hPa at 20°C (read-across from supporting substance (structural analogue or surrogate)
Water Solubility	Moderately soluble (100-1000 mg/L)
Flammability	Not highly flammable
Explosive Properties	No data available
Surface Tension	30.9 mN/m at 20°C
Octanol/water Partition coefficient (Kow)	log K_{OW} = 4.48 at 25°C (estimated value)
Product and Process Description	Alkyl amidopropyl betaine is an amphoteric surfactant and the most common representative of the betaine type surfactants. In the production of alkyl amidopropyl betaine two main steps are involved: formation of the fatty acid amide and carboxy-methylation of the amide. For coco fatty acid amido propyl betaine (CAPB), which is represented here, the first step is the reaction of 3-dimethylaminopropylamine (DMAPA) with either fatty acids, fatty acid methyl esters or directly with natural fats (fatty acid glycerin esters). The predominant source oils used determine the fatty acid composition of the betaine, which corresponds to that of the oil. During the reaction DMAPA is partly distilled from the reaction

	medium together with the released methanol or water. To use DMAPA very efficiently and avoid large amounts of liquid waste the amine is recycled. The amidoamine is carboxymethylated in an aqueous medium with chloroacetic acid or its sodium salt. The reaction leads directly to the betaine, normally obtained as a 30% aqueous solution. Sodium chloride, formed as a co-product, is present in most betaine solutions at a concentration of around 5%. Apart from the reaction with the tertiary nitrogen atom, the chloroacetic acid can also be hydrolyzed in a side reaction to form glycolic acid. The glycolic acid content can reach levels of more than 1% in the betaine solution; however, the level is typically considerably lower (<0.1%) [5].
Application	Alkylamidopropyl Betaines are used as ingredients personal care products and cosmetics such as shampoo, shower, liquid soap, face cleaning, as well as in Home Care products like hand dish, hard surface cleaners, laundry detergents.

Life Cycle Assessment

General Introduction

These Eco-profiles or 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 Eco-profiles 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 CAPB. CAPB is an amphoteric surfactant.

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 CAPB and its main precursors/intermediates.

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	Primary production data for CAPB production was collected from different suppliers in Europe. The geographical representativeness for CAPB was considered 'very good'.
Technological Coverage	The technological representativeness for CAPB was considered 'good'. Figure 1 provides a schematic overview of the production process of CAPB.
Representativeness for market volume	>70% (Represented market volume (in mass) covered by primary data used in ERASM SLE project.)
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 CAPB 100% active substance

Cradle-to Gate System Boundaries

Included	Excluded
Fatty acid methyl ester production (oleo)	Construction of major capital equipment (Infrastructure)
DMAPA production (this production is further explained in the Eco Profile fact sheet of the precursor DMAPA (#26))	Maintenance and operation of support equipment
Chloroacetic acid production (this production is further explained in the Eco Profile fact sheet of the precursor Chloroacetic acid (#27))	Human labor and employee transport
Energy production	Packaging
Utilities	
Transportation processes for the main materials	
Water use and treatment of waste water	
Treatment of wastes	

Assumptions and Limitations		Transportation was only considered for the main materials (covers about 90% of the mass of all inputs), other transportation was not considered. Some important transports were estimated by European standard due to lack of valuable information.
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	Allocation was applied for some background data. Allocation methods used for the renewable precursors PKO and CNO (mass allocation).
	Aggregated data	Vertical averaging was considered (as long as the final product was the same, different processes with common product intermediates can be aggregated in the average).

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.

Primary Energy Demand (PED): An analysis of the inventory data shows that the PED impact is mainly caused production of the precursor DMAPA, which is also one of the main inputs by mass, C8-18 fatty acid methyl ester (32%) and the precursor Chloroacetic acid. The remaining contribution comes from the generation of electricity, the thermal energy and the contribution of other chemicals. The contribution of utilities, transports and the treatment of process waste are negligible.

Global Warming Potential (GWP): An analysis of the inventory data shows that the GWP impact is mainly caused by production of the precursor DMAPA (56%), which is also one of the main inputs by mass. The precursor Chloroacetic acid accounts for 19% of the total GWP. The generation of electricity causes 10% and the thermal energy 9% of the impacts contributing to the global warming potential. The contribution of other chemicals is roughly 6%. The contribution of utilities, transports and the treatment of process waste are negligible.
The C8-18 fatty acid methyl ester, which is one of the main inputs related to mass, has a strong impact on the Global Warming Potential indicator due to fixation of carbon dioxide.

Table 1. Primary Energy Demand and air emissions related to Global Warming per 1 tonne of C8-18 Alkyl Amidopropyl Betaine 100% active substance

LCI result	Unit	Amount
Primary energy demand		
Primary energy demand from renewable materials (net calorific value)	MJ	25004
Primary energy demand from fossil materials (net calorific value)	MJ	51155
Primary energy demand from fossil and renewable materials (net calorific value)	MJ	76159
Air emissions related to Global Warming Potential		
Carbon uptake, biotic	kg CO_2 equiv.	-2886
Carbon dioxide, fossil	kg	2619
Carbon dioxide, biotic	kg	1135
Carbon dioxide, from land use, land use change and peat oxidation	kg	1030
Methane	kg	15
Nitrous oxide (laughing gas)	kg	0.65
NMVOC emissions	kg	2.37
*Total GWP (according to [**IPCC 2007**])*	*t CO_2-equiv.*	*2.46*

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, BioIS by Deloitte Dr. Yannick Schmidt (2.0 LCA Consultants)
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] Zoller, U. *et al*. (2009). Handbook of Detergents: Part F: Production, Volume 142, CRC Press.

Figure1. Production process of C8-18 Alkyl Amidopropyl Betaine.