Date: 02/06/2017

Environmental Fact Sheet (#4)

C12-15 Alcohol (petro)

petrochemical precursor

Substance Identification			
IUPAC Name	Alcohols, C12-13-branched and linear	**CAS Number**	740817-83-8
Other Names			
Molecular Formula	UVCB substance (substances of Unknown or Variable composition, Complex reaction products or Biological materials), no univocal molecular formula available	Structural formula (example): 	

Physical/Chemical Properties (proxy from C12-13 Fatty Alcohol) [1]	
Molecular Weight	186.33 – 228.41 g/mol
Physical state	Liquid
Appearance	Colourless
Odour	Typical odour
Density	0.8348 g/cm3
Melting Points	6 °C at 1atm
Boiling point	265.8 °C at 1atm
Flash Point	140 °C at 1atm
Vapour Pressure	5 Pa at 20°C
Water Solubility	2.7 mg/l at 20 °C
Flammability	Study scientifically unjustified
Explosive Properties	Not contain chemical groups associated with explosive properties
Surface Tension	No data available
Octanol/water Partition coefficient (Kow)	log K_{OW} = 5.4 at 25 °C
Product and Process Description	C12-15 alcohol is an essentially linear surfactant precursor of petrochemical origin. C12-15 alcohol represented in this project is produced from petrochemical feedstock and based on the oxo process. The oxo process (hydroformylation) consists of the reaction of olefins with an H2/CO gas (oxo gas) mixture in the presence of suitable catalysts. The process involves the following steps: oxo reaction, catalyst separation and regeneration, aldehyde hydrogenation and alcohol distillation. [5].
Application	Fatty Alcohols possess good foaming properties and ready biodegradability, and are extensively used as base surfactants for laundry detergent products, shampoo, dishwashing liquids and cleaners.

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 C12-15 fatty alcohol. C12-15 fatty alcohol 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 C12-15 fatty alcohol.

Temporal Coverage	Data for fatty alcohol production was collected as 12 month averages representing the year 2011, to compensate seasonal influence of data. Background data have reference years from 2008 to 2010. The dataset is considered to be valid until substantial technological changes in the production chain occur.
Geographical Coverage	Current data of C12-15 fatty alcohol production were based on three suppliers in Europe. The geographical representativeness for C12-15 fatty alcohol was considered 'good'.
Technological Coverage	The technological representativeness for C12-15 fatty alcohol was considered 'good'. Figure 1 provides a schematic overview of the production process of C12-15 fatty alcohol.
Representativeness for market volume	>80% (Represented market volume (in mass) covered by primary data used in ERASM SLE project).
Declared Unit	In the 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 ton of C12-15 fatty alcohol 100% active substance.
Cradle-to Gate System Boundaries	See table below
Assumptions and Limitations	Mass- and impact-relevant catalysts and other chemicals were estimated by expert judgment, otherwise a cut-off was applied according to the given cut-off rules below. Transportation was only considered for the main materials (covers about 90% of the mass of all inputs), other transportation was not considered.
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.

Included	Excluded
Alpha olefin production	Construction of major capital equipment (Infrastructure)
Energy production	Maintenance and operation of support equipment
Utilities	Human labor and employee transport
Transportation processes for the main materials	Packaging
Water use and treatment of waste water	
Treatment of wastes	

	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	Mass allocation was applied to the foreground system as the by-products of the production system occur up to 15% of the total process output mass. Moreover, allocation was applied for some background data.
	Aggregated data	Average production was not disclosed.
Life Cycle Inventory and Impact Assessment [2]		
LCI data for C12-15 fatty alcohol are not published due to confidentiality reasons. However, the data are integrated in the fatty alcohol ethoxylates and/or sulphates.		

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] Arpe, H.-J. (2010). Industrial Organic Chemistry, 5th Edition, Wiley-VCH Verlag.

Figure 1. Production process of C12-15 Fatty Alcohol (petro).