

Environmental Fact Sheet (#32)

Sodium CocoAmphoAcetate (SCA)

oleo/petrochemical amphoteric surfactant

Substance Identification	
IUPAC Name	Imidazolium compounds, 1-(carboxymethyl)-4,5-dihydro-1-(hydroxyethyl)-2-norcoco alkyl, hydroxides, monosodium salts
CAS Number	68390-66-9
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: $\begin{array}{c} \text{O} \\ \parallel \\ \text{RC} - \text{NH} - \text{CH}_2\text{CH}_2 - \text{N} - \text{CH}_2 \text{COONa} \\ \\ \text{CH}_2\text{CH}_2\text{OH} \end{array}$
Physical/Chemical Properties	
Molecular Weight	No data available
Physical state	No data available
Appearance	No data available
Odour	No data available
Density	No data available
Melting Points	No data available
Boiling point	No data available
Flash Point	No data available
Vapour Pressure	No data available
Water Solubility	No data available
Flammability	No data available
Explosive Properties	No data available
Surface Tension	No data available
Octanol/water Partition coefficient (Kow)	No data available
Product and Process Description	Sodium Cocoamphoacetate (SCA) is an amphoteric surfactant. The synthesis of amphoacetates and amphodiacetates consists of two distinct steps: synthesis of the hydroxyethyl-imidazoline and carboxy-methylation of the imidazoline with sodium monochloroacetate (SMCA). In the first step, the fatty acid ester (based on coconut and/or palm kernel oil) is condensed with amino-ethyl-ethanol-amine (AEEA) at an elevated temperature and reduced pressure. The reaction proceeds stepwise through the amide state, followed by ring closure. The main component detected after this reaction is imidazoline with traces of noncyclic amidoamines. The second stage of the process is the reaction of the imidazoline with caustic and monochloroacetic acid [4].
Application	Sodium cocoamphoacetate is a foam stabilizer, hair conditioner and a surfactant. It is a mild ingredient suitable for use in cleansing products, shower gels, cleansers and hair products.

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 sodium cocoamphoacetate (SCA). SCA is an oleo/petrochemical 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 [1].

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

Goal and Scope of ERASM SLE Project [1]

The main goal was to update the existing LCI inventories [2] for the production of sodium cocoamphoacetate and its main precursors/intermediates.

Temporal Coverage	Data collected represents a 12 month averages of SCA production in 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 are based on three suppliers representing sodium cocoamphoacetate production in Europe. The geographical representativeness for SCA was considered ‘very good’.																			
Technological Coverage	The technological representativeness for SCA was considered ‘very good’. Figure 1 provides a schematic overview of the production process of SCA.																			
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 [2]. Functional Unit: 1 metric tonne of sodium cocoamphoacetate 100% active substance.																			
Cradle-to Gate System Boundaries	<table border="1" style="width: 100%;"> <thead> <tr> <th style="text-align: center;">Included</th> <th style="text-align: center;">Excluded</th> </tr> </thead> <tbody> <tr> <td>Fatty acid methylester production (based on coconut oil and palm kernel oil)</td> <td>Construction of major capital equipment (Infrastructure)</td> </tr> <tr> <td>Chloroacetic acid production (this production is further explained in the Eco Profile fact sheet of the precursor Chloroacetic acid (#27))</td> <td>Maintenance and operation of support equipment</td> </tr> <tr> <td>AEEA production (this production is further explained in the Eco Profile fact sheet of the precursor Aminoethylethanolamine (#31))</td> <td>Human labor and employee transport</td> </tr> <tr> <td>Energy production</td> <td>Packaging</td> </tr> <tr> <td>Utilities</td> <td></td> </tr> <tr> <td>Transportation processes for the main materials</td> <td></td> </tr> <tr> <td>Water use and treatment of waste water</td> <td></td> </tr> <tr> <td>Treatment of wastes</td> <td></td> </tr> </tbody> </table>	Included	Excluded	Fatty acid methylester production (based on coconut oil and palm kernel oil)	Construction of major capital equipment (Infrastructure)	Chloroacetic acid production (this production is further explained in the Eco Profile fact sheet of the precursor Chloroacetic acid (#27))	Maintenance and operation of support equipment	AEEA production (this production is further explained in the Eco Profile fact sheet of the precursor Aminoethylethanolamine (#31))	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		
Included	Excluded																			
Fatty acid methylester production (based on coconut oil and palm kernel oil)	Construction of major capital equipment (Infrastructure)																			
Chloroacetic acid production (this production is further explained in the Eco Profile fact sheet of the precursor Chloroacetic acid (#27))	Maintenance and operation of support equipment																			
AEEA production (this production is further explained in the Eco Profile fact sheet of the precursor Aminoethylethanolamine (#31))	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.	
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 [1]

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 Sodium CocoAmphoacetate 100% active substance

LCI result	Unit	Amount
Primary energy demand		
Primary energy demand from renewable materials (net calorific value)	MJ	20078
Primary energy demand from fossil materials (net calorific value)	MJ	54620
Primary energy demand from fossil and renewable materials (net calorific value)	MJ	74699
Air emissions related to Global Warming Potential		
Carbon uptake, biotic	kg CO ₂ equiv.	-2354
Carbon dioxide, fossil	kg	3007
Carbon dioxide, biotic	kg	894
Carbon dioxide, from land use, land use change and peat oxidation	kg	438
Methane	kg	9.31
Nitrous oxide (laughing gas)	kg	0.60
NMVOC emissions	kg	2.12
<i>Total GWP (according to [IPCC 2007])</i>	<i>t CO₂-equiv.</i>	<i>2.40</i>

Primary Energy Demand (PED): An analysis of the inventory data shows that the PED is mainly caused by the intermediates production. AEEA and chloroacetic acid production together with fatty acid correspond to about 70%. Electricity and thermal energy contributes about 13% of PED, and transport plays a minor role.

Global Warming Potential (GWP): An analysis of the inventory data shows that the GWP is caused by the intermediates production. AEEA and chloroacetic acid production together represent about 64% of the GWP. Electricity and thermal energy contributes about 22% of PED, and transport plays a minor role.

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, BioS by Deloitte Dr. Yannick Schmidt (2.0 LCA Consultants)
References	<p>[1] Schowanek, D. <i>et al.</i> (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.</p> <p>[2] CEFIC-Franklin (1994). Resource and environmental profile analysis of petrochemical and oleo chemical surfactants produced in Europe. Phase II Final Report, Franklin Associates, LTD.</p> <p>[3] 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.</p> <p>[4] Zoller <i>et al.</i> (2009). Handbook of Detergents: Part F: Production, Volume 142, CRC Press.</p>

Figure 1. Production process of Sodium CocoAmphoAcetate.

