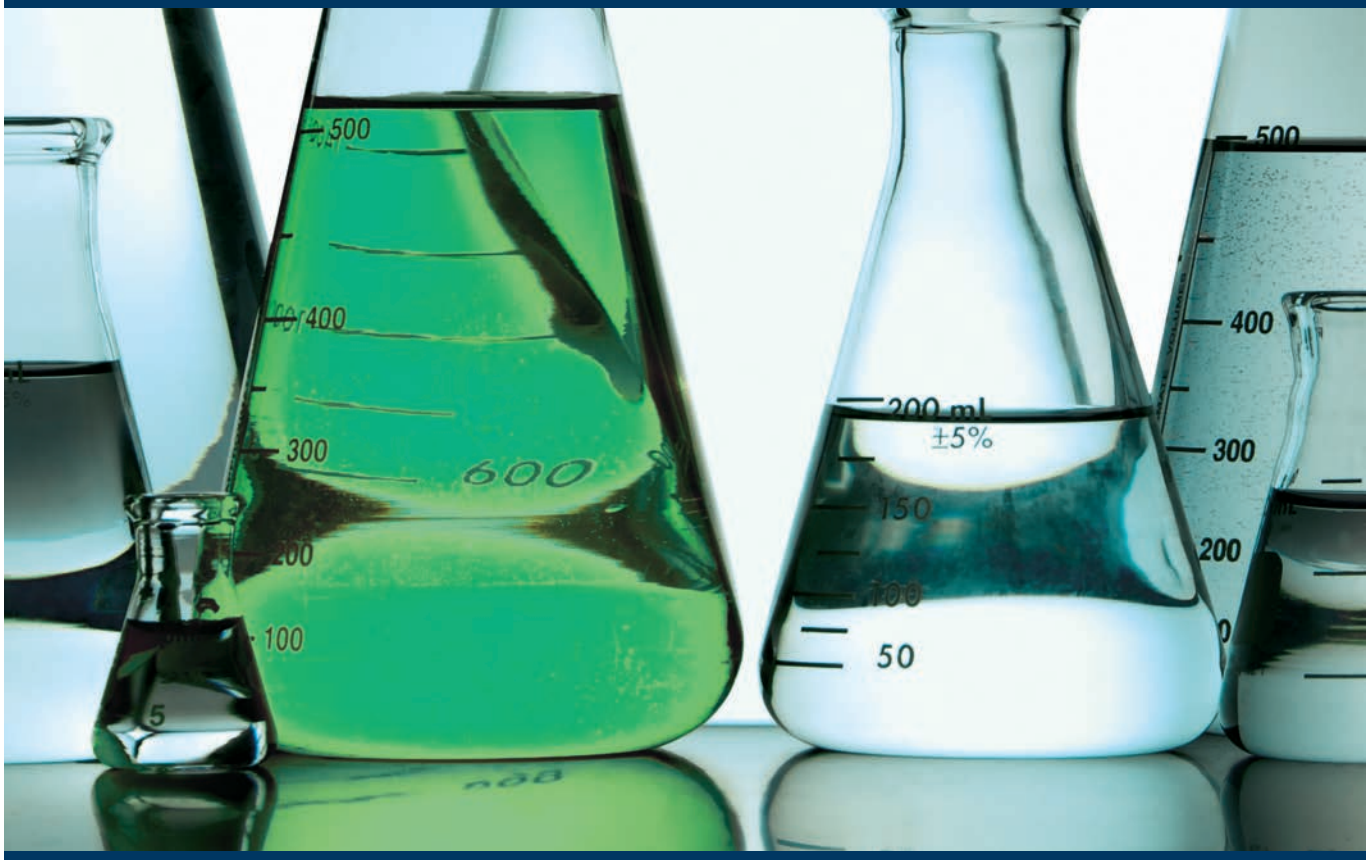
ALCOHOL ETHOXYLATES

Versatile alternatives for technical applications

Sasol Performance Chemicals



Contents

1. About us

Sasol's Performance Chemicals business unit markets a broad portfolio of organic and inorganic commodity and speciality chemicals. Our business employs about 1300 people in four key business divisions: Organics, Inorganics, Wax and PCASG (Phenolics, Carbon, Ammonia and Speciality Gases). Our offices in 18 countries serve customers around the world with a multi-faceted portfolio of state-of-the-art chemical products and solutions for a wide range of applications and industries.

Our key products include surfactants, surfactant intermediates, fatty alcohols, linear alkyl benzene (LAB), short-chain linear alpha olefins, ethylene, petrolatum, paraffin waxes, synthetic waxes, cresylic acids, high-quality carbon solutions as well as high-purity and ultra-high-purity alumina. Our speciality gases sub-division supplies its customers with high-quality ammonia, hydrogen and CO_2 as well as liquid nitrogen, liquid argon, krypton and xenon gases.

Our products are as individual as the industrial applications they serve, with tailor-made solutions creating real business value for customers. Ongoing research activities result in a continuous stream of innovative product concepts that help our customers position themselves successfully in future markets.

Our products are used in countless applications in our daily lives to add value, security and comfort. Typical examples include detergents, cleaning agents, personal care, construction, paints and coatings, leather and metal processing, hot-melt adhesives, bitumen modification and catalyst support for automotive catalysts and other diverse specialty applications including oil and gas recovery, aroma production, plastic stabilisation, and polymer production. Every day, our researchers explore ways to improve our products and develop innovations that improve the quality of people's lives.

2. Introduction / Purpose of this Brochure

Alkylphenol ethoxylates (APEs) are a group of nonionic surfactants that have been popular for more than 40 years due to their effectiveness, economy and ease of handling and formulating. Nonylphenol ethoxylates (NPEs) represent the main product type in this group. They are used mainly in industrial and institutional cleaning, textile and leather processing, metalworking fluids, agrochemicals, emulsion polymerisation, paints, and in a host of smaller applications such as oil field chemicals and paper production.

Within the framework of the Existing Substances Regulation 93/793/EEC, the European Commission has undertaken a comprehensive risk assessment on nonylphenol (NP). NP has been on this list due to the large quantities produced and used annually, its toxicity to aquatic organisms, and concerns that it is not readily biodegradable. NPEs have also been assessed as they are the main pathway of NP to the environment via their biodegradation in the aquatic environment.

The risk assessment, which has been reviewed by the scientific committee of the EU (CSTEE), has been performed for human health and the environment, taking into account all life cycle stages and all environmental media on a local as well as a regional scale. The objective of the EU risk assessment procedure is to assess actual risks as far as possible as well as for scenarios that can be foreseen under “reasonable worst case scenarios”. From the very outset Sasol has been fully involved in this risk assessment, representing the interests of the industry as the biggest European producer of NP and NPEs.

In the risk assessment the major point of concern is the high aquatic toxicity of NP and the possible risks for the aquatic and terrestrial ecosystems. While no human exposure risks were found, the environmental exposure assessment did show clear risks due to aquatic organisms from the acute and chronic toxicities of nonylphenol. The estrogenic effect on humans and the environment was found to be non-risk relevant on the basis of extensive scientific material.

The environmental risk assessment for alkylphenols and their ethoxylates indicated a need to reduce the risks associated with their production, their formulation into other products and the end use of these products in a wide range of industries. In line with the conclusions drawn in the risk assessment the European Commission has demanded the development of a risk reduction strategy proposal addressing the areas of concern.

The course of action taken by the European commission is the proposal for an amendment – the 26th Amendment – to Directive 76/769/EC, the so-called Marketing and Use Directive relating to restrictions on the marketing and use of nonylphenol and nonylphenol ethoxylates for those uses, which have an impact on the aquatic environment.

This 26th Amendment has been published in the Official Journal of the EU on 17 July 2003 and regulates in Annex 1 that nonylphenol and nonylphenol ethoxylates may not be placed on the market or used as a substance or constituent of preparations in concentrations equal or higher than 0.1% by mass for the following purposes:

- Industrial and institutional cleaning except controlled closed dry cleaning systems where the washing liquid is recycled or incinerated or cleaning systems with special treatment where the washing liquid is recycled or incinerated
- Domestic cleaning
- Textiles and leather processing except processing with no release into waste water and systems with special treatment where the washing liquid is recycled or incinerated
- Emulsifier in agricultural teat dips
- Metal working except uses in controlled closed systems where the washing liquid is recycled or incinerated
- Manufacturing of pulp and paper
- Cosmetic products
- Other personal care products except spermicides
- Co-formulants in pesticides and biocides.

After this official publication there is an 18 month transposition period for amending National legislation. Hence from January 2005 on by law nonylphenol and nonylphenol ethoxylates must notbe used any longer in the applications shown above.

3. Alcohol Ethoxylates as Alternatives for Nonylphenol Ethoxylates

Alcohol ethoxylates (FAEs) are the products of choice for the replacement of nonylphenol ethoxylates (NPEs). The performance properties of these nonionic surfactants can be adjusted by the alcohol selection and by the length of the hydrophilic polyethylene glycol chain. In comparison to NPEs, alcohol ethoxylates are usually more biodegradable and their degradation products are unobjectionable in terms of their aquatic toxicity.

In order to find the right alternative product for nonylphenol ethoxylates the functions of these products in the various applications need to be considered. Among the more important features of NPEs are their excellent emulsifying and dispersing properties, which enable the user to very effectively formulate stable emulsions or dispersion concentrates. In the application they act as wetting agents, solubilisers or detergents.

The majority of mid-chain alcohol ethoxylates are even better wetting agents or detergents in most applications. The difficult task for the replacement of NPEs with FAEs is to balance the good wetting and detergency properties with the emulsifying, dispersion and the other properties, which are additionally needed in most applications. Due to the diverse formulation and application requirements, in most cases only the formulator is able to select from among the diverse physical and performance properties of the FAEs to find the right alternative product.

In the following chapter the general properties of industrial alcohol ethoxylates are described to give our customers a guideline for selecting the appropriate FAE.


25 ml
±5%
100
75
50

4. Sasol's Portfolio of Alcohols and Ethoxylates

Sasol Performance Chemicals, as a major producer of alcohols with a total capacity of more than 500,000 t/a C6–22 alcohols, offers numerous differently structured hydrophobes for the production of alcohol ethoxylates. In order to understand the performance characteristics of the alcohols and ethoxylates it is important to discuss briefly the alcohol composition and production processes. Industrial alcohols do not usually consist of only one chemical isomer but are composed of different chemical alcohol structures with variations in alkyl chain length and alkyl branching.

Straight-chain linear alcohols are produced by three different processes:

1. Ziegler process (ALFOL, NAFOL, NACOL)
2. Hydrogenation of oleochemical feedstocks (NAFOL, NACOL)
3. Separation from the oxo alcohols (ALCHEM)

Products comprising a mixture of different alkyl chain length and single cut alcohols are available. Alcohols in the range from C6 to C22 are produced.

The primarily linear- and methyl-branched SAFOL 23 alcohol is produced by the hydroformulation of Fischer-Tropsch olefins derived from coal. The alcohol consists of approximately 55% C12 and 45% C13 carbon chain isomers. The alcohol derivatizes like highly linear alcohol and consists of approximately 50% linear and 50% branched isomers.

LIAL oxo alcohols are derived from the hydroformulation of linear olefins. The LIAL products comprise approximately 45% linear and 55 % branched isomers. Due to the oxo process the branching is always situated in the 2-alkyl position. Sasol separates the completely linear ALCHEM alcohols and the completely branched ISALCHEM alcohols from LIAL by different means.

The multibranched isotridecyl oxo alcohol is produced by the hydroformulation of trimerised butene. It consists of a variety of differently branched C13 isomers. The alcohol is the basis for some of Sasol's surfactant products and is not sold as such.

Monobranched alcohols are derived either from the oxo process, ISALCHEM, or from the Guerbet process, ISOFOL. The ISALCHEM alcohols consist of a set of structural isomers which are all branched in the 2-alkyl position. Products in the range of C11 to C14/C15 are available. ISOFOL alcohols are single isomer products available from C12 up to C32.

Chain length	Straight chain	Straight chain + methyl-branched	Straight chain + mono-branched	Multi-branched	Mono-branched
Oxo process					
C11	ALCHEM 111		LIAL 111		ISALCHEM 111
C12 – C13	ALCHEM 123	SAFOL 23	LIAL 123		ISALCHEM 123
C12 – C15	ALCHEM 125		LIAL 125		ISALCHEM 125
C14 – C15	ALCHEM 145		LIAL 145		ISALCHEM 145
C13 (tri-n-buten based)				Isotridecanol*	
Ziegler process					
C6 – C22 (even numbered)	NACOL types (C6 – C22, single cuts and blends)				
	ALFOL types (C6 – C22+, single cuts and blends)				
Hydrogenation of oleochemical feedstocks					
C12 – C22 (even numbered)	NAFOL types (C12 – C22 blends)				
	NACOL types (C12 – C22 single cuts)				
Guerbet process					
C12 – C32					ISOFOL types

* Isotridecanol is only used for Sasol's alcohol derivatives and is not sold as such.

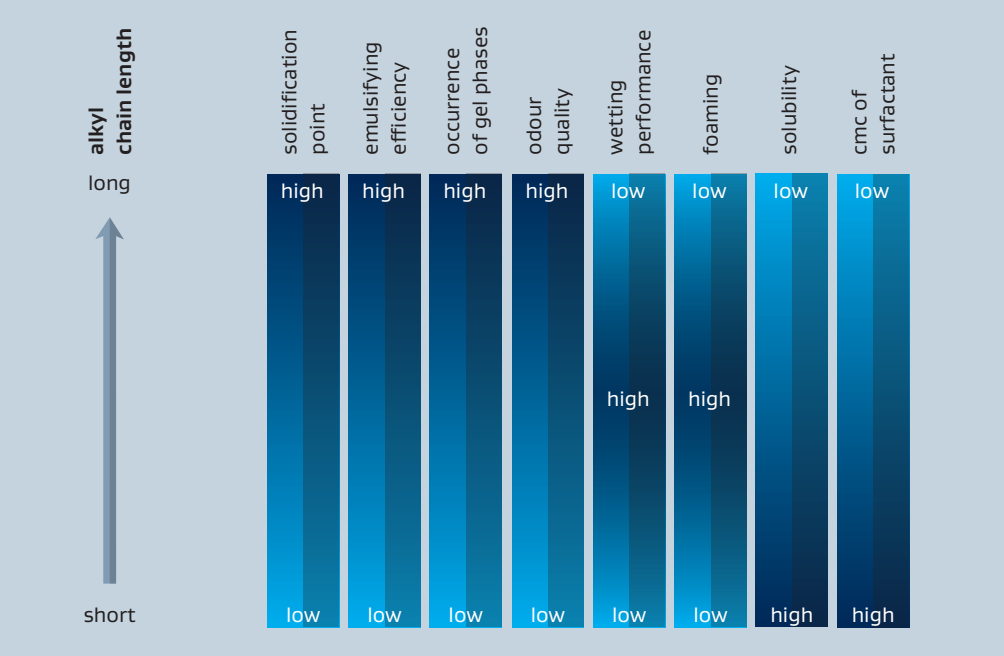
5. Recommendations for Product Selection

The physical and performance properties of alcohol ethoxylates depend on the alkyl chain length, the alkyl branching and the polyethylene glycol chain. Depending on these 3 factors, they demonstrate some general trends in their properties.

5.1 Effects of Alkyl Chain Lengths

A longer alkyl chain results in a higher melting point of the ethoxylates and generally reduced wetting properties if ethoxylation degree and the branching of alkyl chain are kept constant. Foaming is at a maximum for a chain length of about C12 to C13; shorter and longer chained products do not foam as much. Emulsifying efficiency is better for products with a longer alkyl chain, but the occurrence of undesired viscous gel phases also increases with chain length. Longer chain alcohols have a less pronounced odour compared to the shorter chained ones.

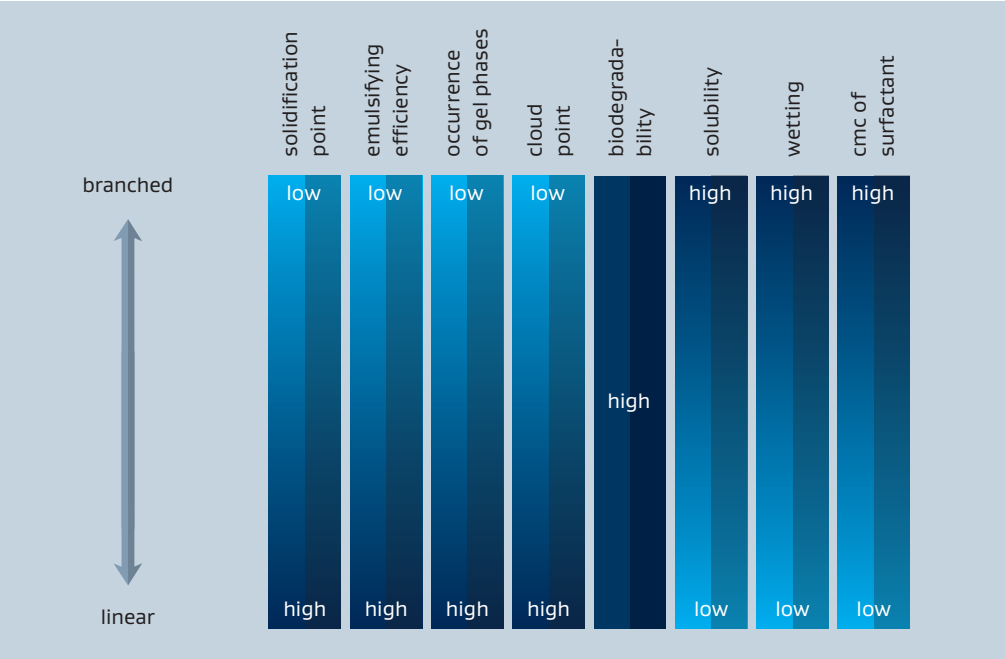
Figure 1:
Schematic representation of the change in surfactant properties due to the alkyl chain length



5.2 Effects of Alkyl Chain Structure

Branching in the alkyl chain causes a lower melting point of the ethoxylates and improved wetting performance if the alkyl chain length and the ethoxylation degree are kept constant. Products with branched chains do not foam as much as straight chain ones under standard conditions. Since the straight chain products have the longest effective chain length and any branching reduces the effective chain length, the linear products show lower critical micelle concentrations and higher emulsifying efficiencies. On the other hand, the more linear products are more prone to produce undesired gel phases if the formulations are not well adjusted. The biodegradation is slightly slower with increased branching.

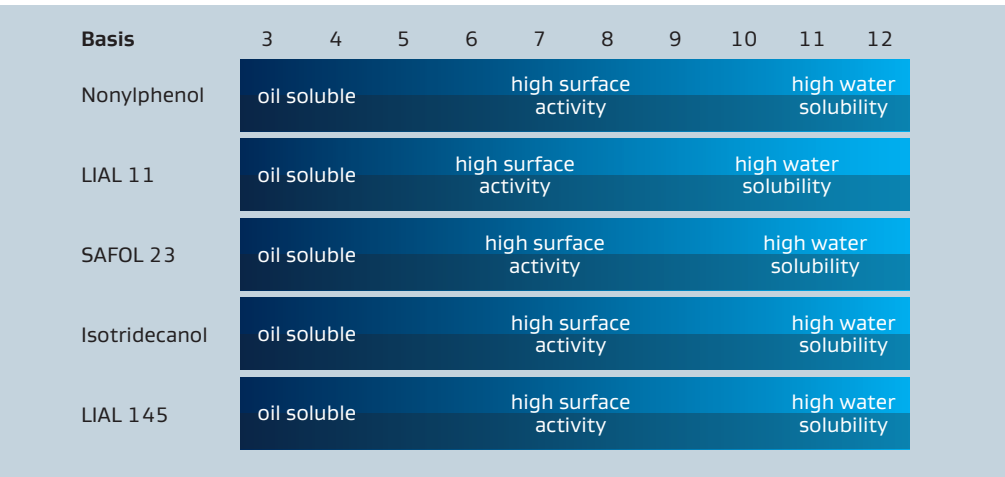
Figure 2:
Schematic representation of the change in surfactant properties due to the branching of the alkyl chain



5.3 Effects of Polyoxyethylene Chain Length

The length of the polyoxyethylene chain is decisive in adjusting the performance characteristics of alcohol ethoxylates. At low ethoxylation degrees the alcohol ethoxylates are oil-soluble. These products are water-in-oil emulsifiers and do not foam in water. Within a medium ethoxylation range the products possess the highest surface activity and best wetting performance. Therefore, these products are multi-purpose surfactants for a wide range of applications. An even higher degree of ethoxylation will further increase the water solubility. Highly ethoxylated products have good dispersing properties and are oil-in-water emulsifiers for hydrophilic oils. Figure 3 depicts the typical order of products with a change in the degree of ethoxylation for some selected alcohols and nonylphenol.

Figure 3:
Schematic representation of the change in surfactant properties due to the degree of ethoxylation



The described performance trends are only a general guide and a starting point for a more detailed discussion. Our technical experts are prepared to discuss your requirements in more detail to find the appropriate solution for your formulations.

6. Technical Data

6.1 NPE alternatives with 3 moles EO

Table of typical product data

Product	Unit	LIALET 111-3	SAFOL 23E2	COSMACOL AE-3	MARLIPAL O13/30	MARLOPHEN NP 3
Based on	—	C11 oxo alcohol LIAL 111	C12/C13 FT oxo alcohol SAFOL 23	C12/C13 oxo alcohol ISALCHEM 123	iso C13 oxo alcohol	nonylphenol
Active Cintent	weight %	100	100	100	100	100
Average Ethoxylation Degree	moles EO	3	2	3	3	3
Average Molecular Weight	g/mol	300	283	326	333	354
HLB (calculated)	—	8.5	6.2	8.1	8.0	7.3.
Appearance at 25 °C	—	cloudy liquid	clear liquid	cloudy liquid	clear liquid	clear. liquid
Cloud Point in water [1]	°C	—	—	—	—	—
Cloud Point in BDG [2]	°C	52	49	47	50	44
Melting / Solidification Point	°C	–9	–12	–3	< –20	< –20
Wetting Value [3]	s	> 300	300	>	300	> 300
Foaming Value at 25 °C [4] (30 s/5 min)	ml	0/0	0/0	0/0	0/0	0/0

[1] 1% in deionised water
[2] 10% in 25% butyldiglycol solution
[3] to DIN EN 1772, time for cotton wetting, 1 g/l, 25 °C
[4] DIN 53917, 1 g/l, 1% in deionised water

6.2 NPE alternatives with 6 moles EO

Table of typical product data

Product	Unit	LIALET 111-5.5	SAFOL 23E5	COSMACOL AE-5	MARLIPAL O13/60	MARLOPHEN NP 6
Based on	—	C11 oxo alcohol LIAL 111	C12/C13 FT oxo alcohol SAFOL 23	C12/C13 oxo alcohol ISALCHEM 123	iso C13 oxo alcohol	nonylphenol
Active Content	weight %	100	100	100	100	100
Average Ethoxylation Degree	moles EO	5.5	5	5	6	6
Average Molecular Weight	g/mol	400	404	414	467	489
HLB (calculated)	—	11.4	10.3	10.6	11.4	10.7
Apperance at 25 °C	—	turbid liquid	turbid liquid	turbid liquid	turbid liquid	clear liquid
Point in water [1]	°C	—	—	—	—	—
Cloud Point	°C	70	71	64	71	69
Melting / Solidification Point	°C	7	3	8	3	< –20
Wetting Value [3]	s	11	17	28	15	42
Foaming Value at 25 °C [4] (30 s/5 min)	ml	65/50	50/30	n.a.	40/30	30/25

[1] 1% in deionised water
[2] 10% in 25% butyldiglycol solution
[3] to DIN EN 1772, time for cotton wetting, 1 g/l, 25 °C
[4] DIN 53917, 1 g/l, 1% in deionised water

6.3 NPE alternatives with 9 moles EO

Table of typical product data

Product	Unit	LIALET 111-7	SAFOL 23E7	COSMACOL AE-7	MARLIPAL O13/90	MARLOPHEN NP 9
Based on	—	C11 oxo alcohol LIAL 111	C12/C13 FT oxo alcohol SAFOL 23	C12/C13 oxo alcohol ISALCHEM 123	iso C13 oxo alcohol	nonylphenol
Active Cintent	weight %	100	100	100	100	100
Average Ethoxylation Degree	moles EO		7	7	9	9
Average Molecular Weight	g/mol	480	510	500	597	621
HLB (calculated)	—	12.8	12.9	12.2	13.3	12.7
Appearance at 25 °C	—	turbid liquid	turbid liquid	turbid liquid	turbid liquid	turbid liquid
Cloud Point in water [1]	°C	54	53	—	56	52
Cloud Point in BDG [2]	°C	—	80	75	—	—
Melting / Solidification Point	°C	14	13	17	13	-5
Wetting Value [3]	s	18	19	19	16	19
Foaming Value at 25 °C [4] (30 s/5 min)	ml	280 /180	170 / 120	n. a.	250 / 150	170 / 130

[1] 1% in deionised water
[2] 10% in 25% butyldiglycol solution
[3] to DIN EN 1772, time for cotton wetting, 1 g/l, 25 °C
[4] DIN 53917, 1 g/l, 1% in deionised water

The products listed in the tables are a selection from a variety of other potential Sasol NPE alternatives. ISOFOL alcohol ethoxylates and NAFOL 810 D based ethoxylates, for example, also offer specific advantages for certain applications.

If you need more detailed information on the product properties and the applications, our sales representatives will put you in touch with our technical service team.

6.4 NPE alternatives with 12 moles EO

Table of typical product data

Product	Unit	LIALET 111-5.5	SAFOL 23E5	COSMACOL AE-5	MARLIPAL O13/60	MARLOPHEN NP 6
Based on	—	C11 oxo alcohol LIAL 111	C12/C13 FT oxo alcohol SAFOL 23	C12/C13 oxo alcohol ISALCHEM 123	iso C13 oxo alcohol	nonylphenol
Active Content	weight %	100	100	100	100	100
Average Ethoxylation Degree	moles EO	10	9	10	12	12
Average Molecular Weight	g/mol	600	584	635	729	753
HLB (calculated)	—	14.3	13.5	13.9	14.5	14.0
Appearance at 25 °C	—	pasty	pasty	pasty	clear liquid	turbid liquid
Point in water [1]	°C	85	81	63	86	81
Cloud Point	°C	—	—	—	—	—
Melting / Solidification Point	°C	25	12	22	-3	12
Wetting Value [3]	s	26	32	28	32	43
Foaming Value at 25 °C [4] (30 s/5 min)	ml	320 / 200	230 / 140	n. a.	310 / 120	320 / 180

[1] 1% in deionised water
[2] 10% in 25% butyldiglycol solution
[3] to DIN EN 1772, time for cotton wetting, 1 g/l, 25 °C
[4] DIN 53917, 1 g/l, 1% in deionised water

At your service

sasol
reaching new frontiers

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