



Dr. Z Presents

All about fatty alcohols

Saturated Fatty Alcohols

Copyright © 2000 by CONDEA

- 2.1 [Physical Properties](#)
- 2.2 [Chemical Properties](#)
- 2.3 [Production Processes](#)
 - 2.3.1 [Production from Natural Sources](#)
 - 2.3.1.1 [Hydrolysis of Wax Esters](#)
 - 2.3.1.2 [Reduction of Wax Esters with Sodium](#)
 - 2.3.2 [Hydrogenation of Natural Raw Materials](#)
 - 2.3.2.1 [Raw Materials and Pretreatment](#)
 - 2.3.2.2 [Hydrogenation Processes](#)
 - 2.3.2.2.1 [Suspension Hydrogenation](#)
 - 2.3.2.2.2 [Gas-Phase Hydrogenation](#)
 - 2.3.2.2.3 [Trickle-Bed Hydrogenation](#)
 - 2.3.3 [Synthesis from Petrochemical Feedstocks](#)
 - 2.3.3.1 [Ziegler-Alcohol-Processes](#)
 - 2.3.3.2 [Oxo-Process](#)
 - 2.3.3.3 [Hydrogenation of Fatty Acids Produced by Oxidation of Paraffinic Hydrocarbons](#)
 - 2.3.3.4 [Bashkirov Oxidation](#)
 - 2.3.3.5 [Other Processes](#)
- 2.4 [Applications](#)

2.1 Physical Properties

Saturated fatty alcohols up to dodecanol are clear, colorless liquids. The next higher homologues are soft materials; tetradecanol and higher alcohols have a waxy consistency. The saturated alcohols crystallize in a nearly orthorhombic lattice [11] and all homologues have a lower specific density than water. The lower homologues have characteristic odors; the higher fatty alcohols are odourless, except for traces of impurities such as carbonyl compounds and hydrocarbons, which are usually present.

Physical properties of linear, primary fatty alcohols are summarized in table 1 (for additional data on pure alcohols and commercially important blends, refer to [12] – [15]).

Table 1: Physical and Chemical Properties of Fatty Alcohols

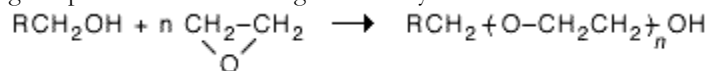
IUPAC name	Common name	CAS registry number	Molecular formula	M	Hydroxyl number	mp °C	bp, °C (p.kPa)
1-Hexanol	caproic alcohol	111-27-3	C ₆ H ₁₄ O	102.2	548	-52	157
1-Heptanol	enanthic alcohol	111-70-6	C ₇ H ₁₆ O	116.2	482	-30	176
1-Octanol	caprylic alcohol	111-87-5	C ₈ H ₁₈ O	130.2	430	-16	195
1-Nonanol	pelargonic alcohol	143-08-8	C ₉ H ₂₀ O	144.3	388	-4	213
1-Decanol	capric alcohol	112-30-1	C ₁₀ H ₂₂ O	158.3	354	7	230
1-Undecanol		112-42-5	C ₁₁ H ₂₄ O	172.3	326	16	245
1-Dodecanol	lauryl alcohol	112-53-8	C ₁₂ H ₂₆ O	186.3	300	23	260
1-Tridecanol		112-70-9	C ₁₃ H ₂₈ O	200.4	280	30	276
1-Tetradecanol	myristyl alcohol	112-72-1	C ₁₄ H ₃₀ O	214.4	261	38	172 (2.67)
1-Pentadecanol		629-76-5	C ₁₅ H ₃₂ O	228.4	245	44	
1-Hexadecanol	cetyl alcohol	36653-82-4	C ₁₆ H ₃₄ O	242.5	230	49	194 (2.67)
1-Heptadecanol	margaryl alcohol	1454-85-9	C ₁₇ H ₃₆ O	256.5	218	54	
1-Octadecanol	stearyl alcohol	112-92-5	C ₁₈ H ₃₈ O	270.5	207	58	214 (2.67)
1-Nonadecanol		1454-84	C ₁₉ H ₄₀ O	284.5	196	62	
1-Eicosanol	arachidyl alcohol	629-96-9	C ₂₀ H ₄₂ O	298.6	187	64	215 (1.33)
1-Heneicosanol		15594-90-8	C ₂₁ H ₄₄ O	312.6	179	68	
1-Docosanol	behenyl alcohol	661-19-8	C ₂₂ H ₄₆ O	326.6	171	71	241 (1.33)
1-Tricosanol		3133-01-5	C ₂₃ H ₄₈ O	340.6	164	74	
1-Tetracosanol	lignoceryl alcohol	506-51-4	C ₂₄ H ₅₀ O	354.7	158	77	
1-Pentacosanol		26040-98-2	C ₂₅ H ₅₂ O	368.7	152	78	

1-Hexacosanol	ceryl alcohol	506-52-5	C ₂₆ H ₅₄ O	382.7	146	81
1-Heptacosanol		2004-39-9	C ₂₇ H ₅₆ O	396.8	141	82
1-Octasanol	montanyl alcohol	557-61-9	C ₂₈ H ₅₈ O	410.8	136	84
1-Nonacosanol		6624-76-6	C ₂₉ H ₆₀ O	424.8	132	85
1-Tricontanol	myricyl alcohol	593-50-0	C ₃₀ H ₆₂ O	438.8	128	87
1-Hentriacontanol	melissyl alcohol	544-86-5	C ₃₁ H ₆₄ O	452.9	124	87
1-Dotriacontanol	lacceryl alcohol	6624-79-9	C ₃₂ H ₆₆ O	466.9	120	89
1-Tritriacontanol		71353-61-2	C ₃₃ H ₆₈ O	480.9	116	
1-Tettratriacontanol	geddyl alcohol	28484-70-0	C ₃₄ H ₇₀ O	494.9	113	92

Boiling points and melting points increase uniformly with increased chain length. Both are significantly higher than those of the hydrocarbons with the corresponding number of carbon atoms. The impact of the polarizing hydroxyl function diminishes with increasing chain length. Thus, hexanol and even octanol show some water solubility, but decanol and the higher fatty alcohols can be considered as immiscible with water. However, a slight hygroscopicity is observed even with octadecanol and higher fatty alcohols, which can absorb water vapor from air during storage. Common organic solvents such as petroleum ether, lower alcohols and diethylether are suitable solvents for fatty alcohols.

2.2 Chemical Properties

The industrial importance of fatty alcohols is based on the large number of reactions the hydroxyl group may undergo. Figure 1 lists some typical examples; many of the resulting derivatives are intermediates of commercial importance, e.g. esters, aldehydes, amines, etc. Ethoxylation with ethylene oxide yields fatty alcohol polyglycol ethers, which are of high importance for the detergent industry:



Under normal conditions, fatty alcohols are resistant to oxidation. However, they can be converted into aldehydes or carboxylic acids using strong oxidants or by catalytic oxidation with air or oxygen [16]–[20]. This reaction is important for the synthesis of C₆–C₁₀ aldehydes if these are not readily available based on natural sources [21] and are therefore produced from synthetic alcohols.

Fatty Alcohol	+ Oxygen	—————>	Aldehyde, Carboxylic Acid
	+ Alkali Melt	—————>	Carboxylic Acids
	+ Alkali	—————>	Dimeric Alcohol
	+ Proton	—————>	Ether, Olefine
	+ Alkyne	—————>	Vinyl Ether
	+ Carboxylic Acid	—————>	Ester
	+ Hydrogen Halide	—————>	Alkyl Halides
	+ Ammonia / Amine	—————>	Amines
	+ Aldehyde / Ketone	—————>	Acetals
	+ Sulfide	—————>	Thiols
	+ Alcoholate / H ₂ S	—————>	Xanthates
	+ Metals	—————>	Metal Alkoxides

2.3.2 Hydrogenation of Natural Raw Materials

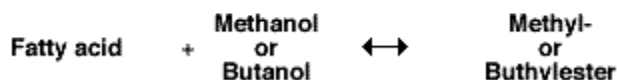
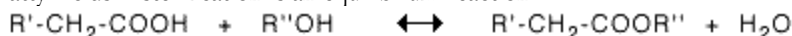
2.3.2.1 Raw Materials and Pretreatment

For the production of C₁₂–C₁₄ alcohols, only coconut oil and palm kernel oil can be used. Palm oil, soybean oil and tallow are the main sources for C₁₆–C₁₈ alcohols. Rapeseed oil rich in erucic acid yields mainly fatty alcohols with 20 or 22 carbon atoms. Bifunctional fatty alcohols can be obtained from castor oil and other special oils ([refer to Chap. 5. Bifunctional Fatty Alcohols](#)).

Before hydrogenation, contaminants such as phosphatides, sterols or oxidation products and impurities such as seed particles, dirt and water are removed in a cleaning process, which includes refining using an adsorption agent. More than 90 % of the vegetable oils are used in food applications.

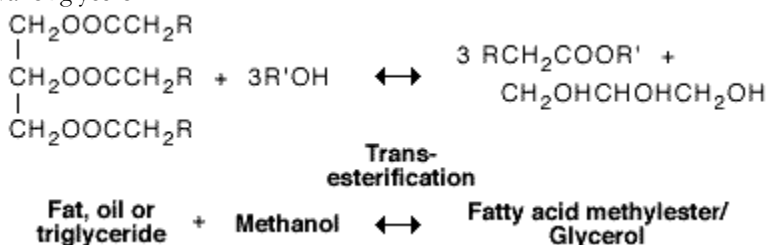
The refined triglycerides are then hydrolyzed to yield fatty acids or transesterified with lower alcohols to yield fatty acid esters. Both refined free fatty acids and fatty acid esters (mostly methyl esters and, more rarely, butyl esters) are used for hydrogenation. Direct hydrogenation of triglycerides is also possible ; however, under the reaction conditions, glycerol is reduced to propylene glycol and propanol and therefore makes no commercial contribution as a by-product. More hydrogen is necessary and catalyst costs increase. Therefore, triglyceride hydrogenation is not used industrially. Fatty acid esters are produced either by esterification of free fatty acids or by transesterification of triglycerides .

Esterification of Fatty Acids. Esterification is an equilibrium reaction:



Excess alcohol or removal of water shifts the equilibrium toward ester formation. Industrial esterification is carried out in a column at 200 – 250°C under slight pressure and with excess methanol. Distilled fatty acids, which no longer have the composition of the original natural product, are predominantly used. Methanol reacts with the fatty acid in a countercurrent. The acid number (milligrams of KOH needed to neutralize one gram of substance) is used as a quality characteristic and for process control. Batch and continuous processes give esters of similar quality, but the continuous process uses less methanol and the residence time is reduced. The methyl ester is subsequently distilled for purification.

Transesterification of Triglycerides. This reaction is carried out continuously with alkaline catalysts. Like esterification, transesterification is an equilibrium reaction and is shifted toward the desired ester by excess methanol or removal of glycerol:



If the reaction is carried out under mild conditions (50 – 70°C, atmospheric pressure, excess methanol), free fatty acids present in the oils must be removed or pre-esterified, e.g. with glycerol first. Under more severe conditions (i.e. at 9 – 10 MPa and 220 – 250°C), pre-esterification is unnecessary, and less pure, cheaper raw materials can be used. Disadvantages of this process are the need for high-pressure equipment, a greater excess of methanol, and the energy-intensive further processing of the aqueous methanol. The methyl esters are purified by distillation. Figure 2 demonstrates the production tree of physical and chemical processing of fats and oils.

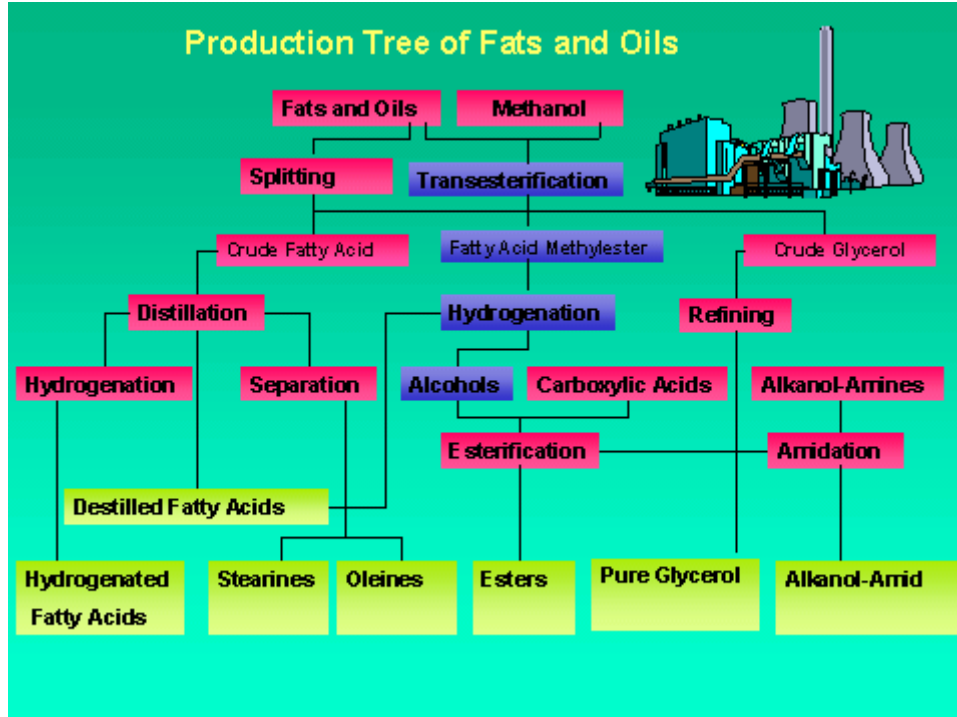


Figure 2: Physical and Chemical Processing of Fats and Oils

2.3.2.2. Hydrogenation Processes

Three large-scale hydrogenation processes are used commercially :

1. gas-phase hydrogenation
2. trickle-bed hydrogenation
3. suspension hydrogenation,

The first two processes use a fixed-bed catalyst. Figure 3 demonstrates a simplified flow diagram. Versus the gas-phase and the trickle-bed hydrogenation the suspension process uses a powdered catalyst with a specific particle size distribution. The selection of the process depends on the integration into existing plants and the choice of raw materials. In all cases, hydrogenation is carried out with copper-containing, mixed-oxide catalysts at 200 – 300°C and 20 – 30 MPa. It was published that Oleofina/B uses a proprietary fixed bed catalyst which operates at 170-250°C and less than 10 MPa (DE 3425758 C2;1984/94).

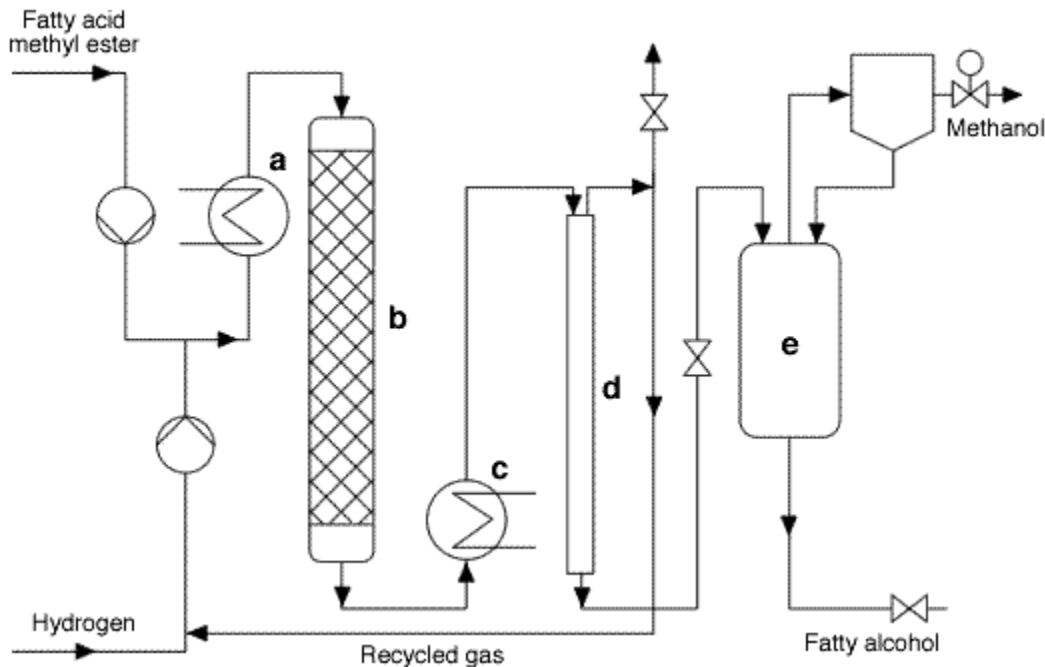


Figure 3:Flow Diagram of the Gas-Phase and Trickle-Bed Hydrogenation of Fatty Acid Methyl Esters a.Heater, b. Reactor, c. Cooler, d. Separator, e. Flash drum

2.3.2.2.1 Suspension Hydrogenation

This process is applicable to fatty acid methyl esters as well as to fatty acids. Hydrogen (ca. 50 mole per mole of ester) and the heated methyl ester are fed separately into the bottom of a narrow reactor. The reaction is carried out at approx. 25 MPa and 250 – 300°C in the presence of a fine powdery copper catalyst ; the LHSV (liquid hourly space velocity) is approximately 1.

The excess hydrogen serves to circulate the reaction mixture. The product mixture is split into a gas phase - which is recycled into the reactor - and a liquid phase, from which the methanol is stripped. The crude product, which still has a saponification number of 6 – 10 (milligrams of KOH required to saponify one gram of substance), is distilled off after removal of the catalyst. If a stainless steel reactor is used, this process can be applied to the direct hydrogenation of fatty acids. In this case, an acid-resistant catalyst is required, and catalyst consumption is increased.

A variant that is particularly suitable for the hydrogenation of fatty acids has been developed by Lurgi (Figure 4) [27] , [28] and is used by several manufacturers [29] . This process employs a large excess of fatty alcohol in the hydrogenation reactor. Hydrogen, fatty alcohol, catalyst slurry and fatty acids are fed separately into the reactor ; the ester forms almost instantaneously [30] and is then hydrogenated in the same reactor in a second, slower reaction step. Hydrogenation is carried out at approx. 30 MPa and 260 – 300°C. Catalyst consumption is 5 – 7 kg / mt fatty acid. The catalyst is separated by centrifugation and the crude fatty alcohol, which has an acid number of <0.1 and a saponification number of 2 – 5, is purified by distillation. The selectivity of the process is > 99%. By continuously replacing part of the spent catalyst, the activity of the copper chromite contact can be maintained constant.

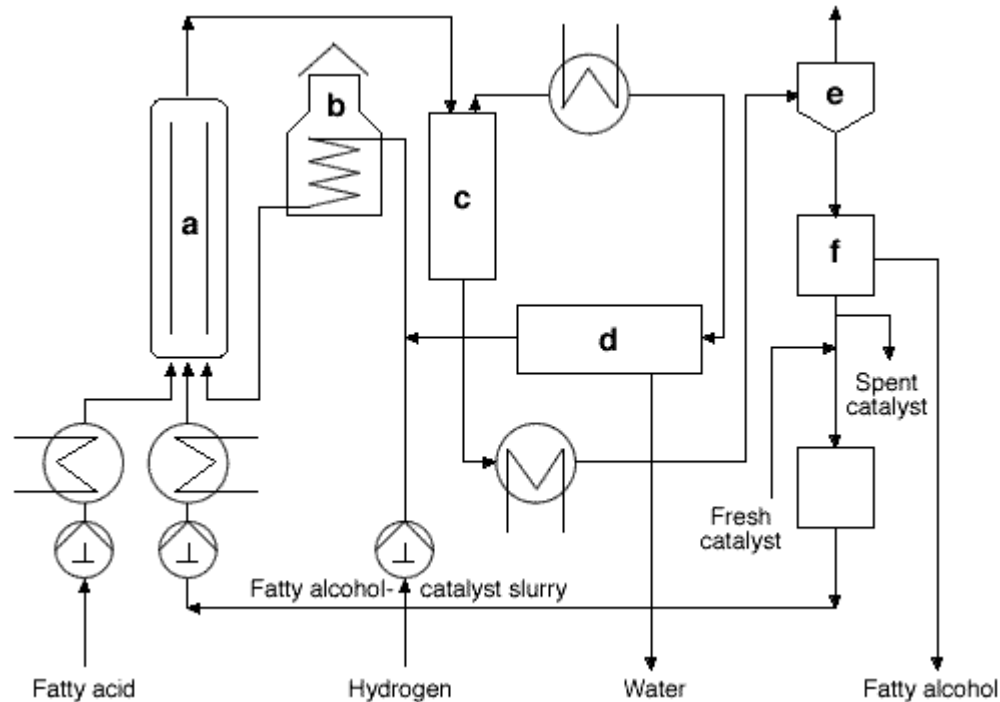


Figure 4: Suspension Hydrogenation of Fatty Acids (Lurgi-Process); a. Reactor, b. Heater, c. Hot separator, d. Cold separator, e. Flash drum, f. Catalyst separation

2.3.2.2.2 Gas-Phase Hydrogenation

This process requires a vaporized substrate and is therefore particularly suitable for methyl esters, preferably with a chain length of 12-14 C-atoms (Figure 3). Characteristics of the process are an extremely large excess of recycle gas (approx. 600 mole of H_2 per mole of ester), high gas velocities and the addition of methanol to aid evaporation [31], [32]. Decomposition of methanol creates significant quantities of carbon monoxide, water and dimethyl ether. Addition of an inert gas to the hydrogen is claimed to make the addition of methanol superfluous and to reduce the excess of recycle gas [33]. Catalysts like copper/zinc or copper/chrome mixed oxides are used in a fixed bed. The conditions required are less than 10 MPa and 230 – 250°C, with a LHSV of about 0.3. Alcohol yields of >99 % are achieved. Catalyst consumption is about 0.3 % based on the feed. The product mixture is split into a gas and a liquid phase; the hydrogen is recycled, the methanol is stripped from the fatty alcohol and the fatty alcohol is purified by distillation. New developments of e.g. Davy McKee (DE 439 5501) should be mentioned. A 30.000 mt/year unit has been constructed by Prime Chem, Philippines.

2.3.2.2.3 Trickle-Bed Hydrogenation.

In this process, the products which are to be reduced are used in their liquid form. It is therefore also suitable for non-vaporizable substrates such as wax esters and fatty acids. Corrosive effects of acids can be avoided by hydrogenation in the presence of amines [34]. If a considerably lower excess of recycle gas (approx. 100 mole of H_2 per mole of ester) is used, a different plant design is necessary. The reaction is carried out at 20 – 30 MPa and about 250 °C, with a LHSV of approx. 0.2. Normally, catalysts are based on copper, chromium- or copper/zinc- mixed oxides. More seldom, supported catalysts like copper chromite on silica are used. Catalyst consumption is about 0.3 % based on the feed. Further treatment of the product is identical to the gas-phase hydrogenation process (refer to fig. 3).

Comparison of Hydrogenation Processes. In the case of the fixed-bed processes (gas-phase and trickle-bed hydrogenation), the catalyst does not need to be separated from the crude fatty alcohol. However, a gradual decrease in the hydrogenation activity due to catalyst poisons such as sulfur, phosphorus or chlorine is

observed, whereas continuous replacement of the catalyst in the suspension process ensures constant activity. If methyl esters are used, separation and further processing of the methanol is necessary. Catalysts that contain noble metals, especially rhenium, may allow hydrogenation at lower pressures, which potentially reduces capital and operating costs [35][36][37]. Further modifications of the processes were developed by Metallgesellschaft (DE 93-4343320) and Davy McKee/Kvaerner (DE 4395501) using wax esters as feed.

2.3.3 Synthesis from Petrochemical Feedstocks

2.3.3.1 Ziegler-Alcohol-Processes

Two processes for the production of synthetic fatty alcohols are based on the work of Prof. Dr. Ziegler using organic aluminum compounds: the ALFOL® process, developed by Conoco, and Ethyl Corporation's EPAL® process [38], [39]. Fatty alcohols synthesized by these processes are structurally identical to natural fatty alcohols and are thus ideal substitutes for natural products.

Conoco started the first ALFOL® plant in the United States in 1962. This plant is now operated by Condea Vista. In 1964 Condea Chemie built a similar plant in Brunsbüttel, Federal Republic of Germany. Ethyl Corporation (today BP/Amoco) developed its own process (EPAL® process) and started operations in 1964. Additional ALFOL® alcohol plants were built in Ufa/ Russia in 1981 and in Jilin/ China in 1998.

ALFOL® Process

Figure (5) shows a simplified diagram of the ALFOL® process [40]. A hydrocarbon is used as solvent. The process involves five steps: hydrogenation, ethylation, growth reaction, oxidation and hydrolysis.

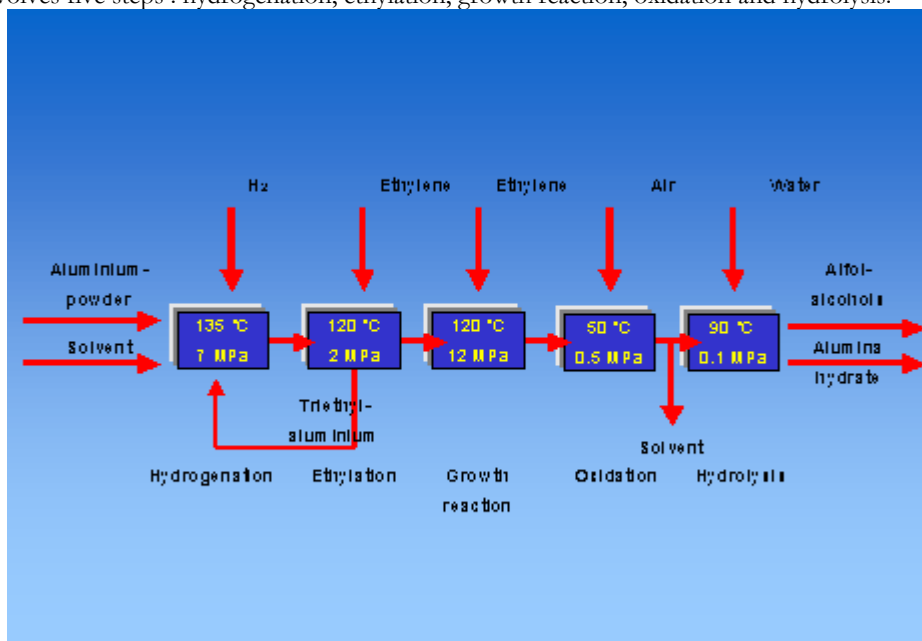
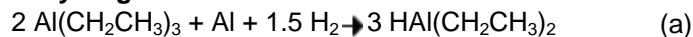
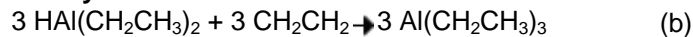


Figure 5: ALFOL®-Alcohol- Process

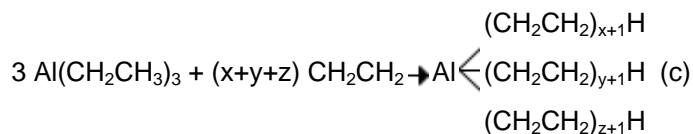
1. Hydrogenation



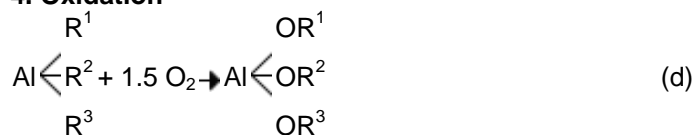
2. Ethylation



3. Growth Reaction



4. Oxidation



5. Hydrolysis

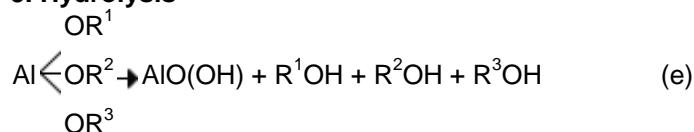


Figure 6: Reaction Steps of the ALFOL®-Process

Two-thirds of the triethylaluminum produced in the ethylation reaction (b) are recycled into the hydrogenation stage (a), and one-third enters the growth reaction (c). Insertion of the ethylene molecule into the aluminum – carbon bonds occurs as a statistical process and leads to a broad distribution (Poisson distribution [41], [42]) of chain lengths, ranging from C₂ to beyond C₂₆ [40]. An optimum yield of the C₁₂ – C₁₄ alcohols, which are important in the surfactant sector, requires addition of about four molecules of ethylene per aluminum – carbon bond (refer to table 1). A small percentage of olefins are formed as by-products.

Due to the varying reactivity of partially oxidized trialkylaluminum compounds, oxidation is carried out stepwise by passing through carefully dried air. Cooling is necessary, especially at the start of the reaction. Alkanes and oxygen-containing compounds are formed as by-products [38].

Prior to hydrolysis, the solvent is removed by distillation. Hydrolysis with water gives high-purity hydrated alumina (PURAL® by CONDEA Chemie GmbH, CATAPAL® by CONDEA Vista Company) as a co-product, which has many industrial applications, e.g. in catalytic processes and ceramics. In the 1960's, hydrolysis was carried out using hot sulfuric acid at Conoco's and Ethyl Corporation's plants. Conoco changed to neutral hydrolysis, but the sulfuric acid method is still used in the EPAL® process and leads to high-purity aluminium sulfate as a co-product. The crude alcohols are finally fractionated into marketable blends and single cuts.

EPAL® Process

Many attempts have been made to achieve a more narrow distribution of chain lengths in the growth reaction [39]. The only process that has been used in an industrial scale is the EPAL® process developed by the Ethyl Corporation (today BP/Amoco). The reaction steps resemble those of the ALFOL® process, but the growth reaction is not carried as far. The product of the growth reaction is subjected to transalkylation (290 °C, 3.5 MPa) with C₄ – C₁₀ olefins. The chain lengths of the resulting trialkylaluminium compounds are predominantly C₄ – C₁₀. Excess olefins are removed in a stripping column and then fractionated. The trialkylaluminium compound is subjected to a second growth reaction and then transalkylated (200 °C, 35 kPa) with C₁₂ – C₁₈ olefins. Again, the olefins are separated in a stripper and fractionated. At this stage, the trialkylaluminium compound consists largely of alkyl chains with 12 – 18 carbon atoms.

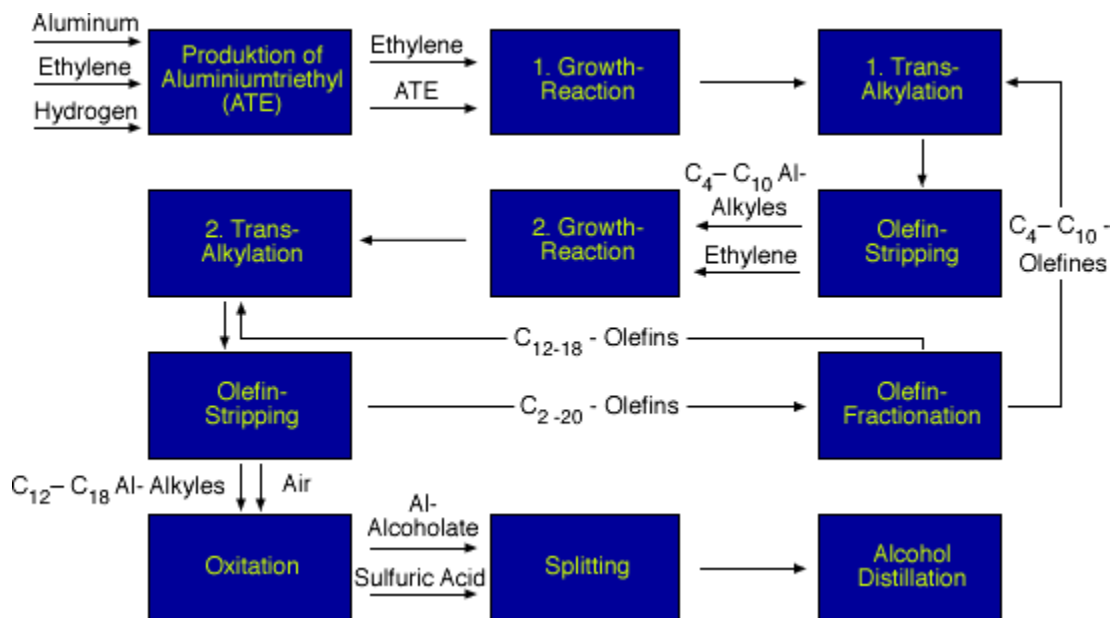


Figure 7: Flow Diagramm of the EPAL®-Process

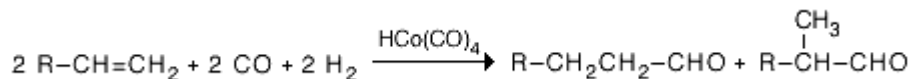
Alcohol	Distribution in %	
	ALFOL®-process	EPAL®-process
Ethanol	0,5	< 0,1
1-Butanol	3,4	0,1
1-Hexanol	9,5	1,5
1-Octanol	16,1	3,5
1-Decanol	19,5	8,0
1-Dodecanol	18,4	34,0
1-Tetradecanol	14,1	26,0
1-Hexadecanol	9,1	16,0
1-Octadecanol	5,1	8,8
1-Eicosanol	2,5	1,9
1-Docosanol	1,1	0,2

Table 2: Typical Alcohol Distribution of the ALFOL®- and EPAL®-Processes

The alcohol distributions resulting from the EPAL® and ALFOL® processes are shown in table (2) [43]. The EPAL® process offers greater flexibility than the ALFOL® process because both the alcohols and the alpha-olefins that are formed as intermediates can be marketed [44]. Disadvantages of the EPAL® process are the higher capital and operating costs, a considerably more complicated process control and an increased proportion of branched olefins and alcohols.

2.3.3.2. Oxo-Process

The Oxo-process (hydroformylation) consists of a reaction of olefins with a H₂/CO gas mixture in the presence of a suitable catalyst. This reaction was discovered in 1938 by O. ROELEN at Ruhrchemie during his work on the Fischer-Tropsch synthesis. Although the first production plant was constructed before 1945 [45], the Oxo-process gained industrial importance only in the 1950's, with the increasing alcohol demand for plasticizers and detergents. The process is based on the following reaction (for details on the reaction mechanism, refer to [46]):



Alpha-Olefins yield approximately equal amounts of linear and branched aldehydes. Internal and branched alkenes can also be used in this reaction. Internal olefins give a product containing some primary aldehydes as the catalyst effects double-bond isomerization.

For a long time, paraffin-based processes were predominant as a source of olefins, especially for detergents [44], [53]. With the development of the SHOP-process (Shell's Higher Olefin Process), ethylene has become the preferred raw material [54]. The principal steps in the SHOP-process are ethylene oligomerization, isomerization and metathesis. The products are C₁₂ – C₁₈ alpha-olefins and C₁₁ – C₁₄ internal olefins, all of which important in the area of surfactants [55], [56].

Heterogeneous hydrogenation of the oxo aldehydes at 5 – 20 MPa and 150 – 250°C in the presence of catalysts based on nickel, molybdenum, copper or cobalt yields the corresponding alcohols. Alternatively, the aldehyde can be subjected to an aldol reaction as in the production of 2-ethylhexanol. Worldwide there are three variants of the Oxo-process [48]: (1) the classical process using HCo(CO)₄ as catalyst; (2) the Shell process based on a cobalt carbonyl – phosphine complex [47]; and (3) a process using a rhodium catalyst. The key parameters of these processes are compared in table 3.

The classical, cobalt-catalyzed Oxo-process involves the following steps: oxo reaction, catalyst separation and regeneration, aldehyde hydrogenation and alcohol distillation. Variants of this process differ mainly in the catalyst separation and regeneration steps [49], [50].

In the Shell process, alcohols are obtained directly due to the greater hydrogenating activity of the catalyst; the aldehyde hydrogenation step is unnecessary. Linearity is improved and the 2-methyl isomer is the main by-product. A disadvantage is the loss of olefins due to hydrogenation to alkanes. Hydroformylation based on a rhodium catalyst has been used by Union Carbide since the 1970's for the production of n-butanol and 2-ethylhexanol [51]. The higher activity of the catalyst enables operation at lower temperature and pressure. For butanol, the linearity is higher than 90%. The disadvantage is the high price of rhodium. For a recent review of the oxo synthesis, refer to [52] by Murrer.

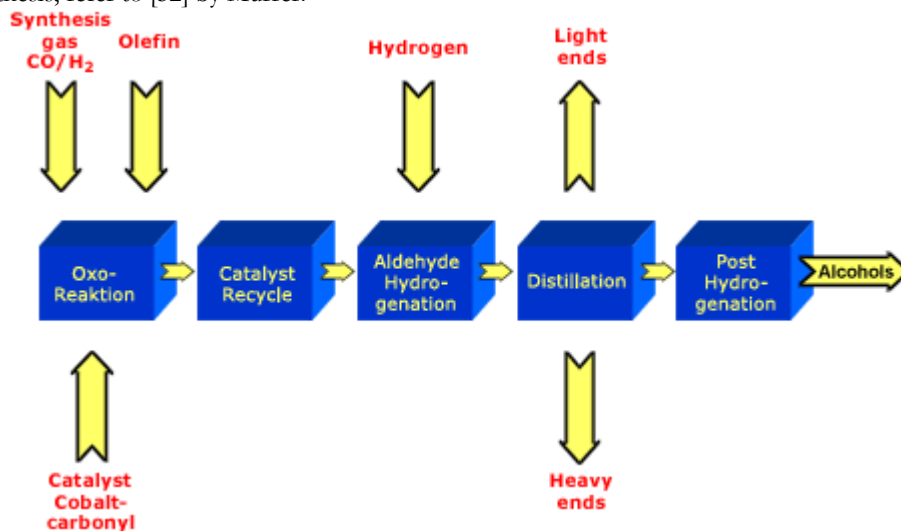


Figure 8: Flow Diagram of the Classical Oxo-Process

Parameter	Oxo-Process		
	Classical	Shell	Union Carbide
Catalyst	Cobaltcarbonyl	Cobaltcarbonyl/ Phosphine complex	Rhodiumcarbonyl/ Phosphine complex
Cat. Conc. %	0,1 — 1,0	approx. 0,5	0,01 — 0,1
CO : H ₂	1:1 — 1,2	1:2 — 2,5	surplus H ₂
Temperature °C	150 — 180	170 — 210	100 — 120

Pressure MPa	20 — 30	5 — 10	2 — 4
LHSV	0,5 — 1,0	0,1 — 0,2	0,1 — 0,25
Primary product	Aldehyde	Alcohol	Aldehyde
Linearity %	40 — 50	80 — 85	approx.90 (Butanol)

Table 3: Typical Process Parameters for the Oxo-Processes

2.3.3.3 Hydrogenation of Fatty Acids Produced by Oxidation of Paraffinic Hydrocarbons

The process for the oxidation of paraffinic hydrocarbons, developed in Germany before 1940, is used in industrial scale in the Eastern European countries, particularly in Russia, for the manufacturing of fatty acids. About 5 – 10 % of these synthetic fatty acids are converted to fatty alcohols. The products are mainly linear, primary alcohols, containing 5 – 15 % branched alcohols. An overview is given in [57]. A mixture of paraffins is oxidized at temperatures above 100 °C in the presence of manganese catalysts. The complex product mixture consists of aldehydes, ketones, esters, carboxylic acids and other compounds. Since the by-products cannot completely be removed during further processing and distillation of the carboxylic acids, the applications of fatty alcohol produced by this method are limited. As for the natural fatty acids, hydrogenation is carried out after esterification using methanol or butanol. The suspension hydrogenation process is used (see Section [2.3.2.2.1 Hydrogenation Processes](#)).

The distillation residue contains esters of C₁₀ – C₂₀ alcohols, 25 % of which are secondary. These alcohols can be obtained by means of hydrolysis.

2.3.3.4 Bashkirov Oxidation

A variant of the paraffinic hydrocarbon oxidation was developed in the 1950's in the former Soviet Union by BASHKIROV [1], [3]. The paraffins are oxidized in the presence of boric acid, which scavenges the hydroperoxides that are formed as intermediates. This results in the formation of boric acid esters of secondary alcohols. These esters are relatively stable to heat and oxidation. Hydrolysis leads to a statistical distribution of secondary alcohols in which the hydroxyl function may occupy any position on the carbon chain. Industrial oxidation is carried out at approx. 160 °C using a nitrogen- air mixture containing approx. 3.5 % of oxygen [58], [59]. The conversion of paraffins is limited to a maximum of 20 % in order to minimize side reactions. The principle reaction steps are demonstrated in the following figure.

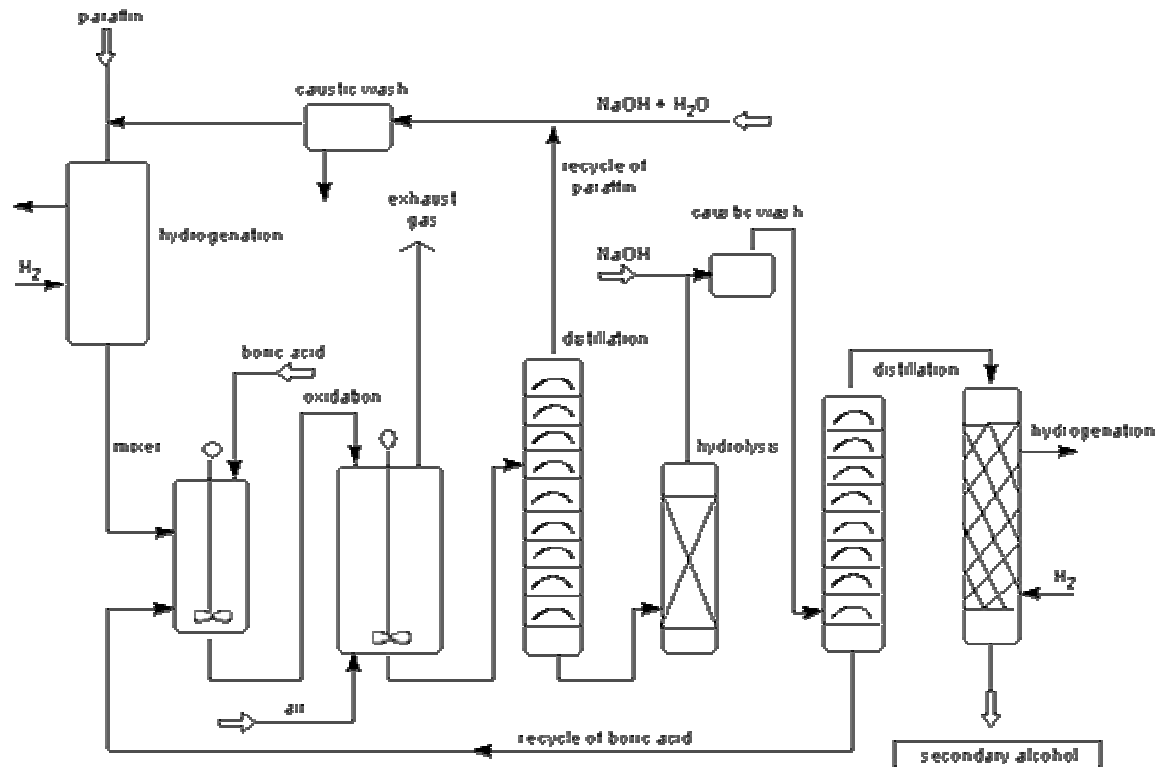
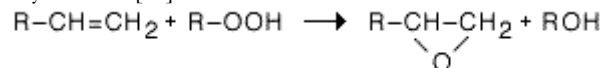


Figure 9: Bashkirov-Oxidation

2.3.3.5 Other Processes

Fatty alcohols can also be obtained by reaction of α -olefins with hydroperoxides in the presence of transition-metal catalysts, especially molybdenum [61]:



If tert-butyl hydroperoxide is used, the coproduct isobutanol can be easily separated from the epoxide. After separation of the low molecular mass alcohols and purification, the epoxide is hydrogenated in the presence of a nickel catalyst in order to form the primary alcohol. About 10 – 15 % of the secondary alcohol and 2 % paraffin are obtained as by-products [62]. Mixtures of linear, primary alcohols with average molecular masses between 400 and 700 (corresponding to a chain length of 30 – 50 carbon atoms) are marketed by Petrolite under the trade name UNILIN® [63]. The hydrocarbon content of these mixtures is approx. 20%. Petrolite oxidizes ethylene oligomers in order to produce oxygen-containing products in industrial scale [64]. 1-Triacontanol, which does not occur in common natural raw materials and is produced only in minute quantities in petrochemical processes such as the ALFOL® process, is of interest due to its ability to stimulate plant growth [65]. Several research groups are investigating synthetic pathways based on low cost raw materials [66][67][68][69][70][71].

2.4 Applications

Fatty alcohols are mainly employed as intermediates. In Western Europe, only 5 % are used directly and approx. 95 % are used in the form of derivatives [72].

The amphiphilic character of fatty alcohols, which results from the combination of a nonpolar, lipophilic carbon chain with a polar, hydrophilic hydroxyl group, confers surface activity upon these compounds. Surfactants account for 70 – 75 % of fatty alcohol production [73].

Due to the described reasons fatty alcohols orient themselves at interfaces, which allows their use in emulsions and micro-emulsions. In cosmetic emulsions (creams, lotions) the main function of the fatty alcohols is to

provide consistency, in technical emulsions they are used as co-surfactants and solution aids.

If the hydroxy group of the fatty alcohols is substituted by other, larger hydrophilic groups, the polar character is enhanced and surfactants are obtained [4]. A short historical overview, as presented in the following figures, shows the importance of surfactants for man, especially in the areas of hygiene, personal care and laundry. The life expectancy of e.g. a laundress in the last century was approx. only 40 years. Thus, the introduction of modern detergents and laundry techniques not only had an impact on the quality of life but on the life expectancy of women as well.

The substances, which are described in the following, can be regarded as the most important fatty alcohol derivatives in the area of surfactants.

Alkyl polyglycoethers (fatty alcohol polyglycoethers, fatty alcohol ethoxilates) were the first nonionic surfactants which were manufactured in technical scale. For the synthesis of this substance class fatty alcohols are reacted with ethylene oxide in a base-catalyzed reaction. In addition, the fatty alcohol alkyleneoxide adducts have to be mentioned, which are also manufactured in a base-catalyzed reaction of fatty alcohols, ethylene oxide and propylene oxide. The latter, in comparison to the first mentioned compounds, are low-foaming surfactants.

Alkylsulfates (fatty alcohol sulfates) belong to the group of anionic surfactants and to the longest known synthetic surfactants. In order to synthesize this class of compounds, fatty alcohols are reacted with SO_3 , chlorosulfonic acid, oleum or sulfuric acid. The resulting semi-esters are subsequently neutralized with an alkali base, mostly NaOH.

Alkyl polyglycoether sulfates (fatty alcohol ether sulfates) also belong to the group of anionic surfactants. For the synthesis, fatty alcohols are reacted with ethyleneoxide and the resulting adducts are caused to react with sulfuric trioxide or chlorosulfonic acid. The subsequent neutralization is usually carried out using caustic soda, ammonia or ethanolamine.

Alkyl methylammonium chlorides belong to the group of cationic surfactants and are produced using fatty alcohols especially in the range of C_{16-18} .

Alkyl polyglucosides (APG) are manufactured from fatty alcohols and sugar molecules following various procedures. They are kind to the skin and, if necessary, can be manufactured from renewable raw materials only. However, high production costs are usually a limiting factor.

In addition, the polar character of the fatty alcohols allows their use as lubricants during the processing of polymers. Esters of the fatty alcohols with fatty acids, so-called wax esters are utilized among other applications as lubricants during the polymer processing and as raw materials for waxes and creams in technical applications. In cosmetic applications esters are used as well, however, here usually the liquid products on the basis of unsaturated fatty alcohols and/or fatty acids are preferred.

Acrylic acid- or methacrylic acid esters of fatty alcohols are precursors of polymethacrylates, which are utilized as flow enhancer and viscosity index improver in crude oils and lubricating oils. For similar applications fumaric acid esters are also used.

Esters on the basis of adipic acid, sebacic acid, trimellitic acid and citric acid as well as phthalic acid esters are used as plasticizers for PVC. The various specific applications of specialty plasticizers is based on their chemical structure, their high cold flexibility, good compatibility, high thermostability, high aging stability and low fogging-values in the finished product. Each of the mentioned esters offers special chemical and physical properties for the different application areas.

A further high volume application is the area of fragrances and flavors. Aldehydes, esters or alkyl groups on the basis of fatty alcohols are sometimes incorporated into more complex molecules of fragrance and flavor essentials. Important for this application are high purity single cuts which can be processed into the mentioned products without any loss in quality.

An additional example, in the area of semi-luxuries, is the cultivation of tobacco. Alcohols with a chain length of C_8-10 are used as so-called tobacco sucker control agents.

Especially fatty alcohols with chain lengths C_{18} and longer have two additional interesting application areas, either in an emulsified form or as derivatives. In a lot of countries water is extremely expensive and rare. During the dry seasons the water reservoirs have to be protected against evaporation. If fatty alcohols are emulsified with interface-active substances, the resulting emulsion can be applied to the water surfaces. The layer, which is formed fast and easily on the water surface, prohibits the evaporation and therefore protects the water reserves. Field tests in Europe and in Africa have proved the effectiveness. The evaporation can be reduced up to 50 %. The need for high quality papers, the modern, fast operating paper machines and the increased ecological requirements demand highly effective paper defoamer systems. Products on the basis of fatty alcohols show the following advantages compared to silicon based defoamers: high effectiveness, good biodegradability, good drainage and deairation, water recycling and high cost effectiveness. Each paper quality and each production facility demands different defoamer qualities, which contain emulsifiers and additives in addition to the alcohol.

All about fatty alcohols

3. Unsaturated Fatty Alcohols

Unsaturated fatty alcohols are special and can only be obtained from natural sources ; petrochemical processes for their manufacturing do not exist. Unsaturated fatty alcohols contain in addition to the hydroxyl function one olefinic group minimum. Therefore they can react both as alcohols and as olefins. The physical and chemical properties of the most important unsaturated fatty alcohols are listed in table 4. The melting points are lower than those of the corresponding saturated alcohols and are influenced by the configuration of the double bond.

Table 4: Physical and Chemical Properties of Primary Unsaturated Fatty Alcohols

IUPAC name	Common name	CAS registry number	Molecular formula	M	Hydroxyl number	Iodine number	mp, °C	bp, °C (p, kPa)
10-Undecen-1-ol		112-43-6	C ₁₁ H ₂₂ O	170.3	329	149	-2	133 (2.1)
(Z)-9-Octadecen-1-ol	oleyl alcohol	143-28-2	C ₁₈ H ₃₆ O	268.4	209	95	- 7.5	208-210 (2.0)
(E)-9-Octadecen-1-ol	elaidyl alcohol	506-42-3	C ₁₈ H ₃₆ O	268.4	209	95	36-37	216 (2.4)
(Z,Z)-9,12-Octadecadien	linoleyl alcohol	506-43-4	C ₁₈ H ₃₄ O	266.5	211	191	-5 to -2	153-154 (0.4)
(Z,Z,Z)-9,12,15-Octadecatrien-1-ol	linolenyl alcohol	506-44-5	C ₁₈ H ₃₂ O	264.5	212	288		133 (0.27)
(Z)-13-Docosen-1-ol	erucyl alcohol	629-98-f	C ₂₂ H ₄₄ O	324.6	173	78	34-35	240-242 (1.3)
(E)-13-Docosen-1-ol	brassidyl alcohol	5634-26-4	C ₂₂ H ₄₄ O	324.6	173	78	53-54	238-243 (1.05)

Production: The first large-scale hydrogenation plant (Henkel) went into operation in the late 1950's. Previously, unsaturated fatty alcohols could be obtained only by hydrolysis of whale oil ([Section 2.3.1.1. Hydrolysis of Wax Esters](#)) or by the Bouveault – Blanc reduction ([Section 2.3.1.2. Reduction of Wax Esters with Sodium](#)).

Today, a broad range of raw materials based on animal or vegetable fats and oils are available. Market factors and the degree of unsaturation (iodine number) required in the final product, both influence the selection. For products with iodine numbers of 50-75, cheap beef tallow or vegetable raw materials are available. Products with iodine numbers of 80-100 can be produced based on technical oleic acid (animal or vegetable based). Polyunsaturated products are undesirable as they tend to autoxidation. For special applications products with higher iodine numbers (> 110) based on sunflower- or soybean oils are produced. Unsaturated alcohols

with iodine numbers >150 are e.g. produced based on linseed oil. These products contain a higher content of unsaturated alcohols by nature.

The hydrogenation processes are described in [section 2.3.3.3](#). Hydrogenation processes are suitable for the large-scale production of unsaturated fatty alcohols. The fixed-bed processes are preferred due to the mild reaction conditions. In suspension hydrogenation, the prolonged contact between fatty alcohol and catalyst results in side reactions such as saturation of the double bond and formation of trans isomers, which leads to a higher solidification point and, hence, loss of quality. With polyunsaturated fatty acids, the formation of conjugated double bonds cannot be prevented completely.

Hydrogenation is generally carried out at 250 – 280°C and a pressure of 20 – 25 MPa. Catalysts include zinc oxide in conjunction with aluminum oxide, chromium oxide, or iron oxide, and possibly other promoters [80][81][82][83][84][85]; copper chromite whose activity has been reduced by the addition of cadmium compounds; and cadmium oxide on an alumina carrier [86]. Selective hydrogenation can also be carried out in a homogeneous phase using metallic soaps as catalysts. An overview on catalyst developments is given in [74]; further references can be found in [75][76][77][78][79]. Recent patent applications indicate great interest in selective catalysts [87][88][89][90][91][92].

Unsaturated fatty alcohols are produced in the Federal Republic of Germany (Henkel, Salim) and in Japan (New Japan Chemical).

Applications: Unsaturated fatty alcohols are used in detergents, in cosmetic ointments and creams, as plasticizers and defoamers and in textile and leather processing [23], [93][94][95]. Oleyl alcohol is also used as an additive in petroleum and lubricating oils.

Copyright © 2000 by CONDEA

All about fatty alcohols

4. Guerbet Alcohols

The condensation of primary alcohols at temperatures of 180 - 300°C in the presence of alkaline condensing agents leads to primary, alpha-branched dimeric alcohols. The difference versus other branched fatty alcohols is shown in figure 10. The physical and chemical properties are listed in table 5.

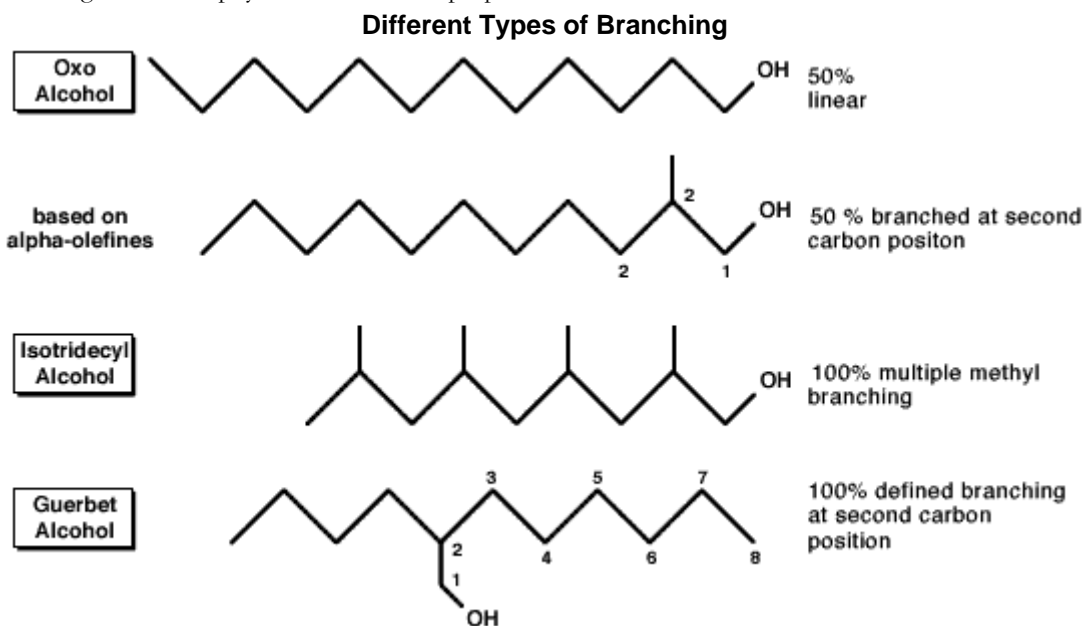


Figure 10: Examples of Different Types of Branched Fatty Alcohols
 Table 5: Physical and Chemical Properties of Guerbet Alcohols

IUPAC name	CAS registry number	Molecular formula	M_r	Hydroxyl number	mp, °C	bp, °C (p, kPa)
2-Methyl-1-pentanol	105-30-6	C ₆ H ₁₄ O	102.18	549	-147.9	149.9 (101.3)
2-Ethyl-hexanol	104-76-7	C ₈ H ₁₈ O	130.23	431	< -76	118 (10.7)
2-Propyl-heptanol	10042-59-8	C ₁₀ H ₂₂ O	158.29	354		117 (2.7)
2-Butyl-1-octanol	3913-02-8	C ₁₂ H ₂₆ O	186.34	301		126-128 (1.5)
2-Pentyl-1-nonanol	5333-48-2	C ₁₄ H ₃₀ O	214.39	262		154 (1.7)
2-Hexyl-1-decanol	2425-77-6	C ₁₆ H ₃₄ O	242.45	231	-30 to -26	175 (1.5)
2-Heptyl-1-undecanol	5333-44-8	C ₁₈ H ₃₈ O	270.50	207	-26	198 (2.0)
2-Octyl-1-dodecanol	5333-42-6	C ₂₀ H ₄₂ O	298.56	188	-20	135-137 (0.007)
2-Nonyl-1-tridecanol	54439-52-0	C ₂₂ H ₄₆ O	326.61	172		164-167 (0.013)
2-Decyl-tetradecanol	58670-89-6	C ₂₄ H ₅₀ O	354.67	158		173-175 (0.007)
2-Undecyl-1-pentadecanol	79864-02-1	C ₂₆ H ₅₄ O	382.72	147		
2-Dodecyl-hexadecanol	72388-18-2	C ₂₈ H ₅₈ O	410.77	137		203-207 (0.007)
2-Tridecyl-heptadecanol		C ₃₀ H ₆₂ O	438.83	128		
2-Tetradecyl-1-octadecanol	32582-32-4	C ₃₂ H ₆₆ O	466.88	120	38-39	308-310 (2.0)
2-Pentadecyl-1-nonadecanol		C ₃₄ H ₇₀ O	494.94	113		
2-Hexadecyl-1-eicosanol	17658-63-8	C ₃₆ H ₇₄ O	522.99	107	43-45	270-280 (0.013)
2-Heptadecyl-1-heneicosanol		C ₃₈ H ₇₈ O	551.05	102		
2-Octadecyl-1-docosanol		C ₄₀ H ₈₂ O	579.11	98		
2-Nonadecyl-1-tricosanol		C ₄₂ H ₈₆ O	607.16	95		
2-Eicosyl-tetracosanol	73761-81-6	C ₄₄ H ₉₀ O	635.22	93		

This reaction, which was first observed by M. Guerbet (96), was thoroughly studied regarding its reaction mechanism and regarding suitable catalysts (3, 5). For further extensive literature please refer to the literature cited here. Figure 11 illustrates the reaction mechanism in simplified terms.

Mechanism of the Guerbet Reaction

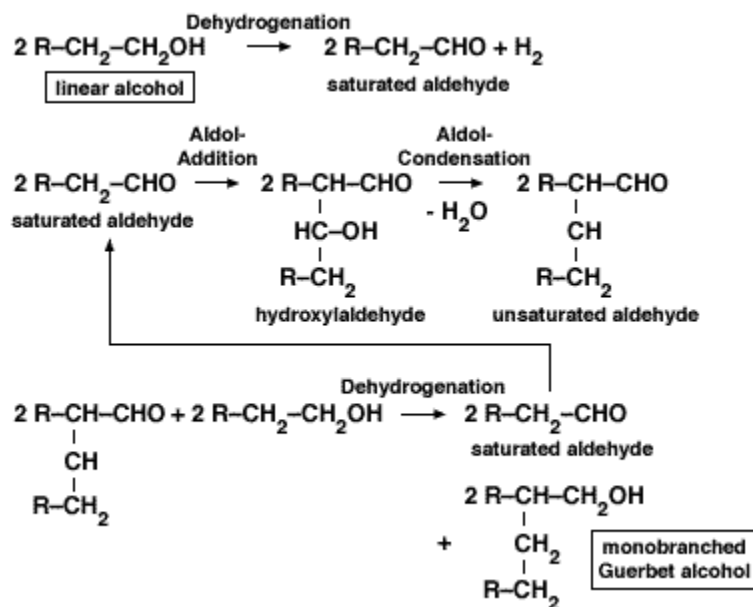


Figure 11: Mechanism of the Guerbet Reaction

Today this reaction is performed in technical scale with a worldwide production capacity of several thousand mt/year. The alcohol which is to be dimerized, is mixed with an alkaline condensing agent and a hydrogenation-/dehydrogenation catalyst and then heated to 180 - 300°C. The formed reaction water is distilled off continuously together with the monomeric alcohol. Since the reaction proceeds faster at higher temperatures, especially the reaction of short-chain monomeric alcohols (C₆-C₁₀-OH) is performed under pressure. However, it has to be considered that low-molecular, alpha-branched dimeric alcohols, like e.g. 2-ethyl-1-hexanol, can be manufactured in a more economic way using other methods (refer to Ullmann, Vol. A1, 279).

The properties and applications of the Guerbet alcohols can be summarized as follows [97]:

By introducing a defined single alkyl-branching the physicochemical properties of the Guerbet alcohols and their derivatives are determined in a characteristic way:

- Melting point or pour point are considerably decreased compared to linear alcohols with the same molecular weight.
- Volatility and vapor pressure are significantly lower compared to linear alcohols with comparable consistency (but lower molecular weight).
- Versus the likewise liquid unsaturated alcohols the Guerbet alcohols have the advantage of a good stability against oxidation and rancidity.

Based on these properties Guerbet alcohols in the range of C₁₂₋₃₆ can be used in the following application areas :

- Cosmetic-pharmaceutical oil components with high stability against autoxidation (rancidity).
- Plasticizers for synthetic resins, e.g. nitrocellulose (for the production of permanent templates).
- Solvents or solution aids for printing colors and specialty inks.
- Lubricant components e.g. for metal processing oils and fiber preparations.
- Components for chemical reactions, e.g. production of branched carboxylic acids.
- Starting materials for textile auxiliaries, e.g. esters, sulfates, phosphates, ethersulfates.

The Guerbet alcohols C₃₂₋₃₆, which can be manufactured from C₁₆₋₁₈-alcohols, are used as:

- Esterification components for the manufacturing of specialty waxes.
- Raw materials for cosmetic stick preparations.

All about fatty alcohols

5. Bifunctional Fatty Alcohols

Some natural oils which contain double bonds, hydroxyl groups, or other functional groups can be converted into long-chain diols. These are usually alpha,omega-diols or diols whose hydroxyl groups lie far apart. Table 6 lists physical and chemical properties of bifunctional fatty alcohols.

Table 6: Physical and Chemical Properties of Bifunctional Fatty Alcohols

IUPAC name	CAS registry number	Molecular formula	M	Hydroxyl number	mp, °C	pb, °C (p, kPa)
1,6-Hexanediol	629-11-8	C ₆ H ₁₄ O ₂	118.17	949	42	134 (1.3)
1,7-Heptanediol	629-30-1	C ₇ H ₁₆ O ₂	132.20	849	18	151(1.9)
1,8-Octanediol	629-41-4	C ₈ H ₁₈ O ₂	146.23	767	61	167-168 (2.4)
1,9-Nonanediol	3937-52-2	C ₉ H ₂₀ O ₂	160.26	700	45	173.2 (1.9)
1,10-Decanediol	112-47-0	C ₁₀ H ₂₂ O ₂	174.29	644	73	175-176 (1.9)
1,11-Undecanediol	765-04-8	C ₁₁ H ₂₄ O ₂	188.31	596	63	178 (1.6)
1,12-Dodecanediol	5675-51-4	C ₁₂ H ₂₆ O ₂	202.34	555	81	183-184 (1.25)
1,13-Tridecanediol	13362-52-2	C ₁₃ H ₂₈ O ₂	216.37	519	75-76	195-197 (1.3)
1,14-Tetradecanediol	19812-64-7	C ₁₄ H ₃₀ O ₂	230.39	487	85	200 (1.2)
1,15-Pentadecanediol	11722-40-8	C ₁₆ H ₃₂ O ₂	244.42	459	70.6-71.6	205-207 (1.3)
1,16-Hexadecanediol	7735-42-4	C ₁₆ H ₃₄ O ₂	258.45	434	91.4	195-200 (0.53)
1,17-Heptadecanediol	6577-59-1	C ₁₈ H ₃₆ O ₂	272.48	412	96-96.5	204-205 (0.27)
1,18-Octadecanediol	3155-43-9	C ₁₉ H ₃₈ O ₂	286.50	392	97-98	210-211 (0.27)
1,19-Nonadecanediol	7268-65-7	C ₂₀ H ₄₀ O ₂	300.53	373	101	212-214 (0.2)
1,20-Eicosanediol	7735-43-5	C ₂₀ H ₄₂ O ₂	314.56	357	102.4-102.6	215-217 (0.2)
1,21-Heneicosanediol	95008-70-1	C ₂₁ H ₄₄ O ₂	328.58	342	105-105.5	223-224 (0.2)
1,22-Docosanediol	22513-81-1	C ₂₂ H ₄₆ O ₂	342.61	328	105.7-106.2	
1,23-Tricosanediol	95491-58-0	C ₂₄ H ₄₈ O ₂	356.64	314		

1,24-Tetracosanediol	22513-82-2	C ₂₆ H ₅₀ O ₂	370.67	302		
1,25-Pentacosanediol	92238-33-0	C ₂₅ H ₅₂ O ₂	384.69	292	109	
(Z)-9-Octadecene	540-11-4	C ₁₈ H ₃₆ O ₂	284.49	394	89	182/0.06

1,2-Diols can be produced by epoxidation of internal or alpha-olefins with subsequent hydrolytic cleavage of the epoxide ring.

Dimerization of unsaturated fatty acids such as soybean, linseed, and tallow fatty acid, followed by esterification and catalytic hydrogenation, results in saturated diols [98].

alpha,omega-unsaturated fatty alcohols can be produced by pyrolysis of castor oil (Atochem) or by metathesis of oleic acid methyl ester (Warwel, PCT/WO96/19287; Noweck PCT/DE/95/01846).

Thermal or catalytic dimerization of unsaturated alcohols yields viscous dimers with complex structure and an average of two hydroxyl groups per molecule [99], [100].

1,12-Octadecanediol, 1,10-decanediol and 9-octadecene-1,12-diol are obtained from castor oil by transesterification and hydrogenation or by alkali splitting, esterification and hydrogenation. Alpha-omega diols with high purity can be produced on purpose from the corresponding dicarboxylic acid esters (DE 38 43956, Hüls AG), e.g.

Suberic acid ester -> 1,8 Octanediol

Sebacic acid ester -> 1,10 Decanediol

Dodecanedioic acid ester -> 1,12 Dodecanediol

Sebacic acid is based on castor oil. Nature offers today new plants and new renewable raw materials by cultivation or genetic engineering.

Bifunctional fatty alcohols are mainly used in the production of polyesters and polyamides and as intermediates.

Copyright © 2000 by CONDEA

All about fatty alcohols

6. Quality Specifications

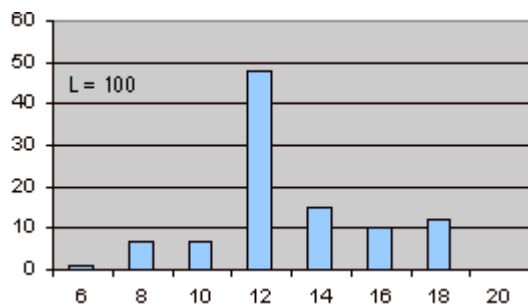
Analytical methods defined by DIN [101] and ASTM [102] standards and by the Deutsche Gesellschaft für Fettwissenschaft (DGF) [103] are used for the quality control of fatty alcohols (refer to table (7)). In addition, analytical methods from the different fatty alcohol suppliers might be used.

The composition of fatty alcohol mixtures is determined by gas chromatography, which can be combined with mass spectrometry. Alcohols from different sources can thus be identified; typical examples are given in figure 12.

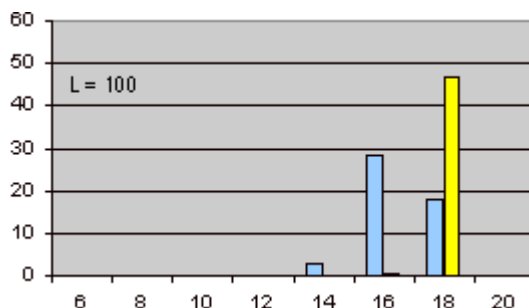
Figure 12: Typical Fatty Alcohol Compositions Obtained by Different Processes

(Blue = n-alcohols; violet=iso-alcohols; yellow=unsaturated alcohols)

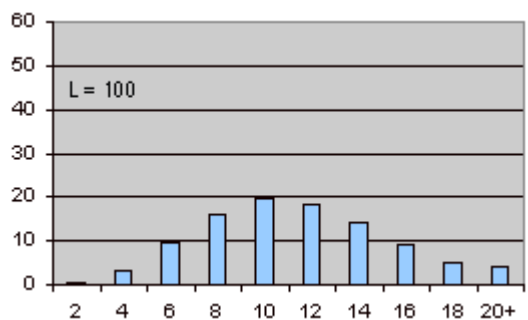
Alcohols Produced by Hydrogenation of Fatty Acid Methyl esters Based on Coconut Oil	Unsaturated Alcohols Based on Vegetable Oils
---	---



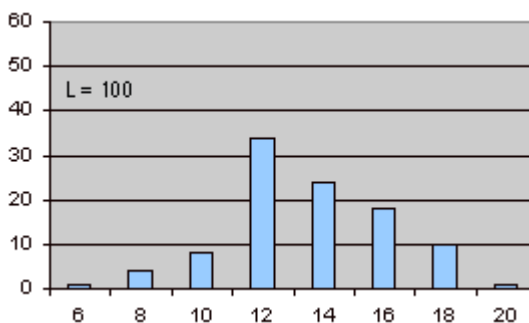
Alcohols from the Ziegler-Alfol-Process



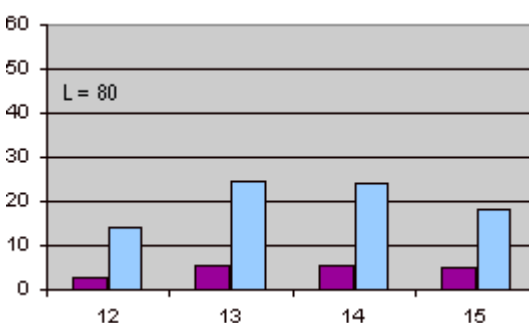
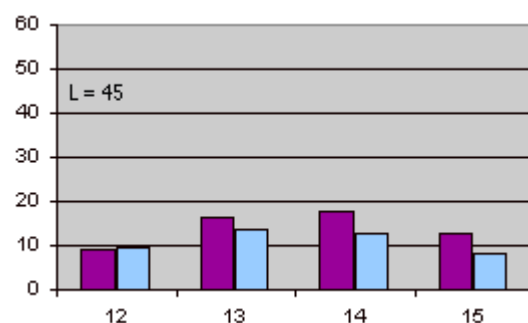
Alcohols from the Ziegler-Epal Process



Oxo Alcohols from Statistical n-Olefins



Oxo Alcohols by Phosphine Catalysis



Linearity L is defined as the percentage of linear alcohols present in the mixture:

$$L = \frac{\text{n - alcohol}}{\text{n - alcohol} + \text{isoalcohol}} \times 100$$

Coconut alcohol gives very few impurity peaks. It contains <0.1 % n-tridecanol and varying amounts of n-alkanes, depending on the hydrogenation process.

Tallow alcohol contains up to 2 % isomeric pentadecanols (isopentadecanol, antepentadecanol, and n-pentadecanol) and n-hexadecane, and up to 4 % isomeric heptadecanols (isoheptadecanol, anteisoheptadecanol, and n-heptadecanol) and n-octadecane.

Ziegler alcohols (Alfol and Epal alcohols) are primary, linear alcohols with an even carbon number. Gas chromatography shows up to 1 % impurities, consisting of numerous even-numbered, isomeric fatty alcohols. Oxo alcohols from statistical, cracked olefins or from paraffin dehydrogenation by the Pacol-process or SHOP-olefins contain a large number of isomers that cannot be completely separated, even with the most efficient capillary columns. Both odd- and even-numbered isoalcohols occur. Oxo alcohol mixtures can be identified by spectroscopic determination of the degree of branching, i.e., the ratio of n-alcohols to isoalcohols, which depends on the production process and the raw materials used.

Fatty acids obtained by oxidation of paraffinic hydrocarbons yield even- and odd-numbered primary alcohols with a low degree of branching. Branched alkanes present in the original paraffins are lost by oxidative degradation. The boric acid-catalyzed process (Bashkirov oxidation) yields secondary alcohols with a statistical distribution of isomers.

Guerbet alcohols are primary, alpha-branched fatty alcohols with two straight-chain alkyl groups of approximately equal length.

Table 7: Analytical Methods for the Characterization of Fatty Alcohols

Analytical method	DGF* (103)	DIN (101)	ASTM (102)
Composition	C-VI 10	By gaschromatography	
Hydrocarbon content		By column chromatography on silica	
Color (Hazen, APHA)		53409 DIN ISO 6271	D 1686-81 D 1209-84
Color (Lovibond)	C-IV 4b		
Refractive-Index	C-IV 5	51423	D 1218-82
Density	C-IV 2b	51757	D 1298-80 D 891-59 (1976)
Viscosity	C-IV 7	51562	D 445-83
Solidification point	C-IV 3c	51570	D 87-77 (1982)
Boiling range		51751	D 1078-83 E 133-78 (1984)
Flash point	C-IV 8	51758	D 56-82 D 93-80
Ignition temperature		51794	D 2155-66 (1976)
Hydroxyl number	C-V 17a	53240	D 1957 (1984)
Carbonyl number	C-V 18		E 411
Peroxide number	C-VI 6a		D 1022-76
Iodine number (Kaufmann)	C-V 11b		
Iodine number (Wijs)	C-V 11 d	53241	D 1959 (1984)
Acid number	C-V 2	DIN EN ISO 3682	D 1613-81
Saponification number	C-V 3	DIN EN ISO 3681	D 94-80
Water content	C-III 13a	51777	D 1744-83
Diol content		Gaschromatography, HPLC, TLC	

* Deutsche Gesellschaft für Fettwirtschaft

Copyright © 2000 by CONDEA

All about fatty alcohols

7. Storage and Transportation

During production, processing and storage, fatty alcohols are handled as liquids. Fatty alcohols starting from C₁₂OH solidify at ambient temperatures. Products with a melting point above 40°C can therefore be transferred to, stored and handled as flakes or pastilles.

Fatty alcohols are sensitive to oxidation and should be stored under an inert gas; the temperature should not exceed 20 °C above the melting point. Low-pressure steam or warm water are recommended for heating. Water increases stability to autoxidation; as little as 0.1 % has a stabilizing effect. The use of antioxidants depends on further processing and quality requirements.

Stainless steel or an Al–Mg–Mn alloy (DIN 1725/1745) are used as container material; ordinary steel should have an inert coating. Pumps, valves, and pipes exposed to the product should be made of stainless steel. For transportation in ships, railroad cars and trucks the same materials should be used .

Fatty alcohols are considered as flammable materials and are classified according to properties such as flash point and boiling point. Their transportation is governed by national and international regulations dealing with volatile and combustible materials.

Copyright © 2000 by CONDEA

All about fatty alcohols

8. Economic Aspects

The economic significance of fatty alcohols is mirrored by the worldwide installed production capacities of approx. 2.0 million mt per year in 1998, which will increase to approx. 2.3 million mt per year by the year 2000. Table 8 shows these production capacities categorized by volume , location and raw materials. In summary, approx. 50 % of the fatty alcohols are produced from natural raw materials, however, the split per geographical region is different from continent to continent. The worldwide production and consumption are estimated at approx. 1.5 million mt per year for 1998. In Europe only approx. 5 % of this volume is used directly as fatty alcohols. A share of 70 - 75 % is used in surfactants exclusively [72, 73, 104-108].

Continent	Production Capacities in 10 ³ Metric Tons		
	Natural Alcohols C ₁₂ and Higher	Synthetic Alcohols C ₁₁ and Higher	Total
USA	170	411	581
Western Europe	408	289	697
Eastern Europe		90	90
Far East	453	162	615
Total	1031	952	1983

Table 8: Estimated Production Capacities for Fatty Alcohols in 1998

In the US the synthetic fatty alcohol capacities predominate with approx. 70 % share of the total capacity. The largest manufacturers of synthetic alcohols are Shell (SHOP/Oxo-process), Amoco (Ziegler/Epal-process) and CONDEA Vista (Ziegler/Alfol-process). Natural fatty alcohols are produced by Procter & Gamble and Henkel. In Western Europe approx. 60 % of the production capacities are based on natural raw materials. The largest manufacturer is the CONDEA Group, using all three technologies, i.e. Ziegler-, Oxo- and natural production processes. The other European manufacturers, like BASF, ICI, EXXON and Shell, predominantly use the Oxo-process. The second largest Western European manufacturer for fatty alcohols, the Henkel Group, manufactures exclusively from natural raw materials using the mentioned high pressure hydrogenation processes.

In the Far East the share of natural production capacities is approx. 75 %. This share will further increase by planned additional capacities of approx. 50,000 mt. The currently largest manufacturers of natural fatty alcohols are the Salim Group and Kao Soap Corp. Synthetic fatty alcohols are manufactured using the Oxo-process among others by Mitsubishi Chemical, Mitsubishi Petrochemical and Fushun or in Jilin using the Ziegler-

process.

In Eastern Europe fatty alcohols are manufactured predominantly on the basis of the paraffin oxidation process.

Considering the existing production capacities and based on the announced capacity increases, assuming an estimated yearly increase of the fatty alcohol demand of 2% to 3%, approx. 80% to 90% of the capacities will be utilized through the year 2005 [72-73, 111, 113].

The planned new capacities will be based on fats and oils and on petrochemical or Fischer-Tropsch raw materials, respectively.

The capacity utilization of each production unit depends on the overall economic development, the product mix and the prices for the used raw materials. Figure 13 shows the differences in price for raw materials based on crude oil, fats and oils.

While until 1973 crude oil based, synthetic fatty alcohol production units had considerable advantages, this picture changed significantly due to the price increases for crude oil in 1973/74 and 1979/80 and subsequently for secondary products like naphtha, paraffins and ethylene. In the long run the price increase rate for fats and oils was considered to be lower than for crude oil [72 - 73, 110 - 111, 114 - 121], leading to an expansion of the natural production capacities. The beginning of 1999 the price for crude oil was close to the price in 1974 again. Therefore, fatty alcohols on the basis of petrochemical raw materials had a raw material cost advantage versus natural based fatty alcohols. This changed again in the second half of 1999.

The long-term estimate was based on higher crop yields for fats and oils, new hybrids, a wider geographical distribution of the cultivation areas and the renewable character of these raw materials versus crude oil. Compared to previous years, all of this guaranteed the supply. Therefore, the ratio of the production capacities of synthetic versus natural fatty alcohols changed in favor of natural products to 1:1 today. The question, however, is not natural or synthetic based fatty alcohols, it is synthetic and natural. However, in spite of production increases for coconut oils, increased utilization of palm kernel and babassu oils and the new hybrids of C₁₂-rich oils like cuphea varieties, nature produces 90 % of all carbon chains in the C₁₆ - C₁₈ range [122]. Synthetic alcohols, however, show their strength especially in the C₁₂ - C₁₅ range, which plays an important role in surfactant applications. Therefore, the C₁₆ - C₁₈ C-chain range is predominantly based on natural, the C₁₂ - C₁₅ range on petrochemical based raw materials. However, due to logistical, economical and political reasons, overlapping and reversals can occur [72,110-111].

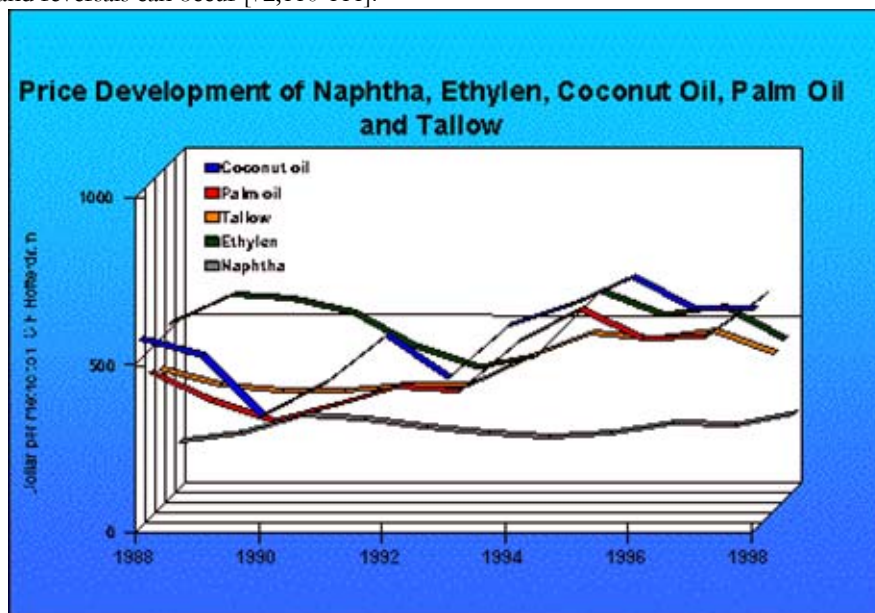


Figure 13: Price Development of Raw Materials Used for the Production of Fatty Alcohols

All about fatty alcohols

9. Ecotoxicology and Toxicology

The following toxicological characterization covers alcohols with C-chain lengths from C₆ to C₂₄. Besides data regarding the acute toxicity (after single intake of the substance) and regarding local effects (skin- and mucous membrane irritation, data on sensitization effects), especially data regarding the toxicity after repeated intake of small amounts of a substance need to be taken into account for the toxicological characterization. This is especially valid for substances which have virtually no acute toxicity as e.g. fatty alcohols. Questions regarding a possible carcinogenic effect or regarding a possible reproduction damage or teratogenic effects are the main focus point today when the toxicological properties of chemical substances are assessed.

For the assessment of the properties of fatty alcohols CONDEA data as well as data from scientific publications were used. Here especially the IUCLID-data were consulted, which were compiled by the manufacturers according to the EG-Altstoffverordnung (EEC 793/93). The data quoted from the IUCLID-data, especially data regarding the acute toxicity, were used without consulting the original publications.

Ecotoxicology/Environmental Properties

Linear fatty alcohols in general are easily biodegradable. As opposed to the linear fatty alcohols the biological degradation of secondary fatty alcohols proceeds slightly slower, however, the decomposition rates in standardized lab tests are comparatively high. For the assessment of the data it has to be considered that the solubility of fatty alcohols in water decreases with an increasing C-chain length. Therefore, the alcohols are present only in an extremely low concentration to show any possible effects. Effects, which are detected in various test systems, often have to be regarded as secondary effects caused by undissolved, finely dispersed substance particles, and therefore have to be distinguished from "real" substance effects.

For aquatic organisms fatty alcohols possess only moderate acute toxicity. In general, in their range of water solubility no toxic effects are observed. However, a number of studies was performed with concentrations which are considerably above the water solubility. The observed toxic effects can also be attributed to the above mentioned secondary effects. The available data for the chronic toxicity do not indicate a special toxicological potential of fatty alcohols as well. Dodecanol shows a more distinct toxicity in the studies. However, this toxicity can not unmistakably be attributed to a direct substance effect, but can possibly be induced by physical effects as well. A complete separation of the aqueous solution from undissolved but finely dispersed dodecanol is virtually impossible. Therefore, a rest of undissolved dodecanol always remains in the water.

Toxicology

In the metabolism linear fatty alcohols are predominantly oxidized. The resulting fatty acids can be integrated into the fatty acid metabolism subsequently. A further metabolic reaction is shown by conjugation reactions with glucuronic acid and subsequent excretion.

Fatty alcohols possess virtually no acute toxicity after oral intake or after exposure to the skin. Especially fatty alcohols with a shorter C-chain length irritate the skin in higher concentrations, in animal tests eye irritations were observed as well. The irritating effect decreases with increasing C-chain length. In studies with volunteers some fatty alcohols show a considerably lower skin irritating effect. This has, at least in part, to be attributed to the different test conditions of studies with volunteers versus animal experiments. The available data as well as the chemical structure of fatty alcohols do not indicate a sensitizing potential of fatty alcohols. Even after long-term intake of the typical linear fatty alcohols from today's point of view, substance induced damage is not to be expected. The available data show that fatty alcohols do not possess a genetic toxicity. This, however, is not to be expected due to their chemical structure. Valid data regarding a carcinogenic effect are not available. But it can be assumed that fatty alcohols do not have a carcinogenic potential based on structure-effect-considerations.

For some of the fatty alcohols at least orientating data regarding a reproduction toxicity are available. These data show that under the study conditions fatty alcohols neither reduced the fertility nor had an embryo- or fetotoxic effect.

In table 9 the data regarding the toxicity after short-term exposure are summarized. Table 10 summarizes the data regarding the acute toxicity against aquatic organisms and degradability data. The above summarized results and the data given in the tables are based upon an extensive number of scientific publications [123-338]. For detailed results regarding the individual fatty alcohols or blends of fatty alcohols please refer to the particular publication.

Table 9: Acute Toxicity (Oral and Dermal), Skin Irritation, Eye Irritation, Sensitization (Data from Animal Experiments)

Substance	LD ₅₀ (oral)	LD ₅₀ (dermal)	Skin Irritation	Eye Irritation	Sensitization
1-Hexanol	3100 - 5000 mg/kg (rat)	1500 -> 5000 mg/kg (rabbit)	Moderately irritant	Irritant	No sensitization
1-Octanol	> 3200 -> 5000 mg/kg (rat)	> 5000 mg/kg (rabbit)	Moderately irritant	Irritant	No sensitization
Decanol	5000 mg/kg (rat)	> 3500 mg/kg (rabbit)	Irritant	Irritant	-
Dodecanol	> 5000 mg/kg (rat)	> 8300 mg/kg (guinea pig)	(Moderately) irritant	(Moderately) irritant	-
Tetradecanol	5000 - 20000 mg/kg (rat)	> 5000 mg/kg (rabbit)	Slightly irritant	Slightly irritant	-
Hexadecanol	> 5000 - > 7500 mg/kg (rat)	> 5000 mg/kg (rabbit)	-	-	No sensitization
Octadecanol	> 5000 - > 8000 mg/kg (rat)	-	-	-	-
Eicosanol	> 10000 mg/kg (rat)	-	Not irritant	Slightly irritant	-
Docosanol	> 10000 mg/kg (rat)	-	Not irritant	Slightly irritant	-
2-Butyloctanol	27 - 33 g/kg	-	Not irritant	Not irritant	No sensitization (human data)
2-Hexyl-1-decanol	> 33000 mg/kg (rat)	-	Slightly irritant	Not irritant	No sensitization (human data)
C₁₆ - C₂₀-Branched Alcohols	> 39000 mg/kg (rat)	-	Not irritant (rabbit)	Not irritant (guinea pig)	No sensitization (guinea pig, human data)
2-Octyldodecanol	> 5000 - > 42000 mg/kg (rat)	-	Slightly irritant (guinea pig)	Slightly irritant (guinea pig)	No sensitization (guinea pig, human data)
2-Decyltetradecanol	> 39000 mg/kg (rat)	-	Not irritant	Not irritant	No sensitization (human data)

Table 10: Ecotoxicity

Substance	Bio-Degradability	Acute Fish Toxicity	Acute Daphnia Toxicity	Algae Toxicity	Bacteria Toxicity
1-Hexanol	Biodegradable	> 100 mg/L	> 100 mg/L	10 - 100 mg/L	3000 - 10000 mg/L
1-Octanol	Biodegradable	10 - 100 mg/L	10 - 100 mg/L	10 - 100 mg/L	350 - > 10000 mg/L
Decanol	Easily biodegradable	1 - 10 mg/L	1 - 10 mg/L	-	> 10000 mg/L
Dodecanol	Easily biodegradable	< 1 mg/L	< 1 mg/L	< 1 mg/L	> 10000 mg/L
Tetradecanol	Biodegradable	-	-	-	-
Hexadecanol	Biodegradable	-	-	> 100 mg/L	-
Octadecanol	Biodegradable	> 100 mg/L	> 100 mg/L	> 100 mg/L	> 10000 mg/L
Eicosanol	-	-	-	-	-
Docosanol	-	-	-	-	-
2-Butyloctanol	Biodegradable	-	-	-	-
2-Hexyl-1-decanol	Easily biodegradable	> 100 mg/L	-	-	-
C ₁₆ - C ₂₀ -Branched Alcohols	-	-	-	-	-
2-Octyldodecanol	Biodegradable	> 100 mg/L	-	100 mg/L	> 10000 mg/L
2-Decyltetra-decanol	Biodegradable	-	-	-	-

Copyright © 2000 by CONDEA

All about fatty alcohols

10. References

10.1 References for chapter 1 through 8

- 1 Ullmann, 4th ed., II, 427-445; 5th ed, vol. A10, 277-256
- 2 ACS Symp. Ser. 159 (1981).
- 3 F. Korte (ed.): Methodicum Chemicum, vol. 5, Stuttgart 1975.

- 4 H. Stache, Tensid Taschenbuch, Carl Hanser Verlag, München 1981.
- 5 Houben-Weyl, VI/1a/b, 1ff.
- 6 Fettalkohole, 2nd ed, Henkel, Düsseldorf 1982.
- 7 H. Adkins, K. Folkers, J. Am. Chem. Soc. 53 (1931) 1095-1097.
- 8 W. Normann, Angew. Chem. 44 (1931) 714-717.
Böhme Fettchemie GmbH, DE 617542, 1930 (W. Normann, H. Prückner);
DE 639 527, 1930 (W. Normann).
- 9 W. Schrauth, O. Schenk, K. Stickdorn, Ber. Dtsch. Chem. Ges. 64 (1931) 1314-1318.
- 10 O. Schmidt, Ber. Dtsch. Chem. Ges. 64 (1931) 2051-2053.
- 11 D. Precht, Fette, Seifen, Anstrichm. 78 (1976) no. 4, 145
- 12 Alfol-Alkohole, Typische Analysendaten, Condea Chemie, Brunsbüttel.
- 13 VDI-Wärmeatlas, Düsseldorf 1984.
- 14 D'Ans Lax-Taschenbuch für Chemiker und Physiker, vol. II, Springer Verlag, Berlin 1964.
- 15 CRC Handbook, 55th ed., -Cleveland 1974/75.
- 16 Houben-Weyl, E3, 265-300.
- 17 Houben-Weyl, E5/1, 202-212.
- 18 K. Heyns, L. Blasejewicz, Tetrahedron 9 (1960) 67.
- 19 E. S. Gore, Platinum Met. Rev. 27 (1983) no. 3, 111
- 20 Atlantic Richfield Co., US 3 997 578, 1976 (Ming Nan Sheng).
- 21 Kirk-Othmer, 9, 795 ff.
- 22 U.R. Kreuzer, J. Am. Oil Chem. Soc. 61 (1984) no. 2, 343.
- 23 H.-D. Komp, M. P. Kubersky in: Fettalkohole, 2nd ed., Henkel, Düsseldorf 1982, p.51 ff.
- 24 E.F. Hill, G.R. Wilson, E. C. Steinle, Jr., Ind. Eng. Chem. 46 (1954) 1917.
- 25 M.L. Karstens, H. Peddicord, Ind. Eng. Chem. 41 (1949) 438.
- 26 H. Igo, CEER Chem. Econ. Eng. Rev. 8 (1976) no. 3, 31
- 27 H. Buchold, Chem. Eng. (N.Y.) 90 (1983) no. 4, 42.
- 28 Th. Voeste, H. Buchold, J. Am. Oil Chem. Soc. 61 (1984) no. 2, 350.
- 29 Chem. Ind. (Düsseldorf) 32 (1980) 739.
- 30 Metallgesellschaft AG, DE 2 853 990, 1978 (Th. Voeste, H.-J. Schmidt,
F. Marschner).
- 31 Dehydag GmbH, DE 1 005 497, 1954 (W. Rittmeister).
- 32 Dehydag GmbH, US 3 193 586, 1965 (W. Rittmeister).
- 33 Henkel KGaA, DE-AS 2 613 226, 1976 (G. Demmering).
- 34 VEB Deutsches Hydrierwerk Rodleben, DD 213 430 1983
(H. Aring, K. Busch, P. Franke, G. Konetzke et al.)
- 35 Institut Français du Pétrole, DE-OS 3 217 429, 1982 (R. Snappe, J.-P. Bournonville).
- 36 B.C. Triverdi, D. Grote, Th. O. Mason, J. Am. Oil Chem. Soc. 58 (1981) no. 1, 17.
- 37 Ashland Oil, Inc. US 4 104 478, 1978 (B.C. Triverdi).
- 38 Houben-Weyl, 13/4, 1ff.

- 39 T. Mole, E.A. Jeffery; *Organoaluminium Compounds*, Elsevier, Amsterdam 1972.
- 40 A. Lundeen, R. Poe: "Alpha-Alcohols", in J.J. Mc Ketta, W.A. Cunningham (eds.): *Encyclopedia of Chemical Processing and Design*, vol. 2, Marcel Dekker, New York 1977, p. 465.
- 41 K. Ziegler, H.-G. Gellert, K. Zosel, E. Holzkamp et al. *Justus Liebigs Ann. Chem.* 629 (1960) 121.
- 42 H. Wesslau, *Justus Liebigs Ann. Chem.* 629 (1960) 198.
- 43 P.H. Washecheck, *ACS Symp. Ser.* 159 (1981) 87.
- 44 K.L. Lindsay "Alpha-Olefins" in J. J. Mc Ketta, W. A. Cunningham (eds.): *Encyclopedia of Chemical Processing and Design*, vol. 2, Marcel Dekker, New York 1977, p. 482.
- 45 *Produkte aus der Oxosynthese*, Ruhrchemie AG, Frankfurt 1969.
- 46 J. Falbe: *Synthesen mit Kohlenmonoxid*, Berlin 1967.
- 47 R.E. Vincent, *ACS Symp. Ser.* 159 (1981) 159.
- 48 B. Cornils, *Compend. Dtsch. Ges. Mineralölwiss. Kohlechem.* 78/79 (1978) no. 1, 463.
- 49 B. Cornils, "New Syntheses with Carbon Monoxide" *React. Struct. Concepts Org. Chem.* 11 (1980).
- 50 H. Lemke, *Hydrocarbon Process.* 45 (1966) no. 2, 148.
- 51 C.E. O'Rourke, P.R. Kavasmaneck, R.E. Uhl, *ACS Symp. Ser.* 159 (181) 71.
- 52 B.A. Murrer, J.H. Russel, *Catalysis* 6 (1983) 169.
- 53 A.H. Turner, *J. Am. Oil Chem. Soc.* 60 (1983) no. 3, 623.
- 54 R.L. Banks, *Appl. Ind. Catal.* 1984, no. 3, 215
- 55 E.R. Freitas, C.R. Gum, *Chem. Eng. Prog.* 75 (1979) 73.
- 56 E.L.T. M. Spitzer, *Seifen, Oele, Fette, Wachse*, 107 (1981) no. 6, 141.
- 57 H. Stage, *Seifen, Oele, Fette, Wachse* 99 (1973) no. 6/7, 143; no. 8, 185; no. 9, 217; no. 11, 299.
- 58 N. Kurata, K. Koshida, *Hydrocarbon Process.* 57 (1978) 145.
- 59 N.J. Stevens, J.R. Livingstone, Jr. *Chem. Eng. Prog.* 64 (1968) no. 7, 61.
- 60 N. Kurata, K. Koshida, H. Yokoyama, T. Goto, *ACS Symp. Ser.* 159 (1981) 113.
- 61 L. Marko, *J. Organomet. Chem.* 283 (1985) 221.
- 62 (62)B. N. Bobylev, M. J. Faberov, S. A. Kesarev, *Khim. Promst. (Moscow)* 1979 no. 3, 1386
- 63 Unilin, *Alcohols*, Petrolite Corp., St. Louis 1985.
- 64 Petrolite Corp., US 4 426 329, 1984 (J.H. Woods, C.E. Laughlin, T.R. Graves).
- 65 S.K. Ries, V. Wert, C.S. Sweely, R.A. Leavitt, *Science* 195 (1977) 1339.
- 66 J. Penninger, M. Biermann, H.-J. Krause, *Fette, Seifen, Anstrichm.* 85 (1983) no. 6, 239.
- 67 T. Gibson, L. Tulich, *J. Org. Chem.* 46 (1981) no. 9, 1821.
- 68 A.V. Rama Rao, J. S. Yadav, G.D. Annapurna, *Synth. Commun.* 13 (1983)

no. 4, 331.

- 69 (69)S.M. Kulkarni, V.R. Mamdapur, M.S. Chadha, Indian J. Chem. Sect. B 22 (1983) no. 7, 683.
- 70 U.T. Bhalerao, S. J. Rao, B.D. Tilak, Tetrahedron Lett. 25 (1984) no. 47, 5439.
- 71 G. Kirchner, H. Weidmann, Liebigs Ann. Chem. 1985, no. 1, 214.
- 72 H.J. Richter, J. Knaut, J. Am. Oil Chem. Soc. 61 (1984) no. 2, 160-175.
- 73 J. Knaut, H.J. Richtler, J. Am. Oil. Chem. Soc. 62 (1985) no. 2, 317.
- 74 H. Bertsch, H. Reinheckel, K. Haage, Fette, Seifen, Anstrichm. 66 (1964) 763.
- 75 H. Bertsch, H. Reinheckel, K. Haage, Fette, Seife, Anstrichm. 71 (1969) 357, 785.
- 76 H. Bertsch, K. Haage, H. Reinheckel, Fette, Seifen, Anstrichm. 71 (1969) 851.
- 77 K. Lindner: Tenside, Textilhilfsmittel, Waschrohstoffe, vol. I, 2nd ed., Wissenschaftl. Verlags GmbH, Stuttgart 1964, p. 144.
- 78 J. Richter: Dissertation, TH Delft 1968.
- 79 J.W.E. Coenen, Fette, Seifen, Anstrichm. 77 (1975) 431.
- 80 Dehydag, US 3 193 586, 1965 (W. Rittmeister)
- 81 Henkel, US 3 729 520, 1973, (H. Rutzen, W. Rittmeister).
- 82 Henkel, DE-AS 2 513 377, 1975 (G. Demmering, H. Schütt, H. Rutzen).
- 83 J. Cieslar, W. Bulanda, Przem, Chem. 63 (1984) 375; Chem. Abstr. 101 (1984) 153 810t.
- 84 Institute Blachownia and Nitrogen Works Kedzierzyn, PL 118 880, 1978 (E. Fabisz, K. Chmielewski, A. Jakubowicz, A. Mankowski et al.).
- 85 Institute Blachowina and Nitrogen Works Kedzierzyn, PL 118 979, 1978 E. Fabisz, K. Chmielewski, A. Jakubowicz, A. Mankowski et. al.).
- 86 New Japan Chemical Ltd., GB 1 335 173, 1972.
- 87 VEB Deutsches Hydrierwerk Rodleben, DD 213 429, 1983, (H. Aring, K. Busch, P. Franke, G. Konetzke et al.).
- 88 UOP Inc., US 4 340 546, 1982 (G. Qualeatti, D. Germanas).
- 89 UOP Inc., US 4 446 073, 1984 (G. Qualeatti, D. Germanas).
- 90 Kao Soap, JP 58 210 035, 1983 (K. Kokubo, K. Tsukada, Y. Miyabata, Y. Kazama).
- 91 Kao Soap, JP 5 995 227 , 1984 (K. Tsukada, Y. Miyabata).
- 92 Kao Soap, JP 59 106 431, 1984 (K. Tsukada, Y. Miyabata, K. Fukuoka).
- 93 H. Schütt in W. Foerst, H. Bucholz-Meisenheimer (eds.): Neue Verfahren, Neue Produkte, Wirtschaftliche Entwicklung; Urban und Schwarzenberg, München 1970.
- 94 U. Ploog, Seifen, Oele, Fette, Wachse 109 (1983) no. 8, 225.
- 95 R.R. Egan, G.W. Earl, J. Ackermann, J. Am. Oil Chem. Soc. 61, 1984, no. 2, 324.
- 96 M. Guerbet, C.R. Hebd. Séances Acad. Sci. 128 (1898) 511; M. Guerbet, Bull. Soc. Chim. Fr. 21 (1899) no. 3, 487.
- 97 J. Glasl in: Fettalkohole, 2nd ed., Henkel, Düsseldorf 1982, p. 169.
- 98 Henkel & Cie GmbH, DE-OS 1 768 313, 1971 (H. Rutzen).

- 99 Henkel & Cie GmbH, DE 1 198 348, 1961 (W. Stein, M. Walther).
- 100 Henkel & Cie GmbH, DE 1 207 371, 1963 (H. Hennig, W. Stein, M. Walther).
- 101 "Mineral- und Brennstoffnormen," DIN-Taschenbuch, Beuth-Vertrieb, Berlin-Köln-Frankfurt 1984.
- 102 Annual Book of ASTM Standards, Sections 5, 6, 15, 1985.
- 103 Deutsche Einheitsmethoden zur Untersuchung von Fetten, Fettprodukten und verwandten Stoffen, Wissenschaftl. Verlag GmbH, Stuttgart, 1950-1984.
- 104 H.J. Richtler, J. Knaut, Chem. Ind. (Düsseldorf) 36 (1984) 131-134.
- 105 H.J. Richtler, J. Knaut, Chem. Ind. (Düsseldorf) 36 (1984) 199-201.
- 106 L. Marcou, Rev. Fr. Corps. Gras. 30 (1983) no. 1. 3-6.
- 107 J. Am. Oil Chem. Soc. 58 (1981) no. 11, 873-874A.
- 108 A.L. de Long, J. Am. Oil Chem. Soc. 60 (1983) no. 3, 634-639.
- 109 Kirk-Othmer, 1, 740-754.
- 110 E.C. Leonard, J. Am. Oil Chem. Soc. 60 (1983) no. 6, 1160-1161.
- 111 C.A. Houston, J. Am Oil Chem. Soc. 61 (1984) no. 2, 179-184.
- 112 J. Am. Oil Chem. Soc. 62 (1985) no. 4, 668.
- 113 J.C. Dean, Chem. Week, 1985, May 15, 3-34.
- 114 J.W. E. Coenen, J. Am. Oil Chem. Soc. 53 (1976), no. 6, 382-389.
- 115 H. Klimmek, Chem. Ind. (Düsseldorf) 33 (1981) 136-141.
- 116 H. Fochem, Fette, Seifen, Anstrichm. 87 (1985) no. 2, 47-52.
- 117 Chem. Week 1982, April 28, 40-44.
- 118 Chem. Ind. (Düsseldorf) 35 (1983) 251-255.
- 119 J. Am. Oil Chem. Soc. 61 (1984) no. 8, 1298-1314.
- 120 H. Lindemann, Chem. Ind. (Düsseldorf) 34 (1982) 713-716.
- 121 S. Field, Hydrocarbon Process. 1984, Oct., 34G-N.
- 122 W. Stein, Fette, Seifen, Anstrichm. 84 (1982) no. 2, 45-54.

10.2 References for chapter 9

- 123 CONDEA Report, unpublished (1987): Acute Oral Toxicity in Rats, NACOL 6 RD, LPT Report 11. Februar 1987.
- 124 Bär, E. und Griepentrog, F. (1967): Medizin Ernähr. 8, 244, cited in: Opdyke, D.L.J. (1975): Fd. Chem. Toxicol. II, 695-696.
- 125 Henkel-Report, unpublished, Arch.-Nr.: TBD 910457, cited in IUCLID Data Set "Hexan-1-ol", compiled for "EG-AltstoffV", 1998.
- 126 CONOCO Report, unpublished (1965): Acute Oral Toxicity (LD₅₀) in Rats, ALFOL 6 Alcohol, Scientific Associates, Inc..
- 127 CONOCO Report, unpublished (1977): Acute Oral Toxicity (LD₅₀) in Rats, ALFOL 6 Alcohol, Scientific Associates, Inc..
- 128 Anonymous (1969): South African Medical Journal. (Medical Assoc. of South

- Africa), 43, 795, cited in Registry of Toxic Effects of Chemical Substances (RTECS), April 1999.
- 129 Henkel-Report, unpublished, Arch.-Nr.: TBD 910457, cited in IUCLID Data Set"Hexan-1-ol", compiled for"EG-AltstoffV", 1998.
 - 130 CONOCO Report, unpublished (1977): Acute Dermal Toxicity (LD₅₀) in Rabbits, ALFOL 6 Alcohol, Scientific Associates, Inc..
 - 131 CONOCO Report, unpublished (1980): Acute Dermal Toxicity (LD₅₀) in Rabbits, ALFOL 6 Alcohol, Scientific Associates, Inc..
 - 132 Smyth, H.F. et al. (1951): Arch. Ind. Hyg., 4, 119.
 - 133 CONDEA Report, unpublished (1986): Acute Skin Irritation/Corrosion Test (Patch Test) of NACOL 6 RD in the Rabbit, LPT Report 17. November 1986.
 - 134 CONOCO Report, unpublished (1965): Acute Dermal Toxicity (LD₅₀) in Rabbits, ALFOL 6 Alcohol, Scientific Associates, Inc..
 - 135 Guido, J. und Martens, M. (1987): Skin and Eye Irritation Tests on Hexanol, J. Am. Coll. Toxicol., Vol. 11(6), 722.
 - 136 CONDEA Report, unpublished (1986): Eye Irritation Study of NACOL 6 RD in the Rabbit after Single Instillation into the Conjunctival Sac, LPT Report 18. Dezember 1986.
 - 137 CONOCO Report, unpublished (1965): Acute Eye Irritation in Rabbits, ALFOL 6 Alcohol, Scientific Associates, Inc..
 - 138 CONOCO Report, unpublished (1982): Primary Eye Irritation in Rabbits, ALFOL 6 Alcohol, Hazleton Raltech, Inc..
 - 139 European Centre for the Ecotoxicology and Toxicology of Chemicals (ECETOC) (1992): Technical Report No. 48, Eye Irritation: Chemicals Reference Data Bank.
 - 140 Henkel-Report, unpublished, Arch.-Nr.: TBD 790129, cited in IUCLID Data Set"Hexan-1-ol", compiled for"EG-AltstoffV", 1998.
 - 141 Henkel-Report, unpublished, Arch.-Nr.: TBD 910457, cited in IUCLID Data Set"Hexan-1-ol", compiled for"EG-AltstoffV", 1998.
 - 142 CONOCO Report, unpublished (1966): Final Report on the Thirteen-Week Subacute Feeding of ALFOL 6 to Rats, Scientific Associates, Inc., Report No. 821.
 - 143 CONOCO Report, unpublished (1966): Final Report on the Thirteen-Week Subacute Feeding in Beagle Dogs of ALFOL 6, Scientific Associates, Inc., Reprot No. 822.
 - 144 Henkel-Report, unpublished, Arch.-Nr.: TBD 900320, cited in IUCLID Data Set"Hexan-1-ol", compiled for"EG-AltstoffV", 1998.
 - 145 Sice, J. (1966): Toxicol. Appl. Pharmacol. 9, 70-74.
 - 146 Nelson, B.K. et al. (1989): J. Am. Coll. Toxicol. 8(2), 405-410.
 - 147 Rodwell, D.E. et al. (1988): The Toxicologist 8(1), 213.
 - 148 Henkel-Report, unpublished, Final Report 882633, cited in IUCLID Data Set"Hexan-1-ol", compiled for"EG-AltstoffV", 1998.
 - 149 CONDEA Vista Report, unpublished (1994): Biodegradability of eleven VISTA ALFOL Alcohols, Technical Service Report 6940-10-05-94.
 - 150 Brooke, L.T. et al. (1984): Acute Toxicities of Organic Chemicals to Fathead

- Minnow (*Pimephales promelas*). Center for Lake Superior Environmental Studies, University of Wisconsin, Vol. 1, WI: 414.
- 151 (151)Veith, G.D. et al. (1983): Estimating the Acute Toxicity of Narcotic Industrial Chemicals to Fathead Minnow. In: W.E. Bishop, R.D. Cardwell, and B.B. Heidolph (Eds.), Aquatic Toxicology and Assessment, 6th Symposium, ASTM STP 802, 90-97.
 - 152 Linden, E. et al. (1979): The Acute Toxicity of 78 Chemicals and Pesticide Formulation against Two Brackfish Water Organisms, The Bleak (*Alburnus alburnus*) and the Harpacticoid, *Chemosphere* 8, No. 11/12, 843-851.
 - 153 Wellens, H. (1982): Comparison of the Sensitivity of *Brachydanio rerio* and *Leuciscus idus* by Testing the Fish Toxicity of Chemicals and Wastewaters. *Z. Wasser Abwasser Forsch.* 15(2), 49-52.
 - 154 Henkel-Report, unpublished, Final Report 882633, cited in IUCLID Data Set "Hexan-1-ol", compiled for "EG-AltstoffV", 1998.
 - 155 Bringman, G. und Kühn, R. (1982): Results of Toxic Action of Water Pollutants on *Daphnia magna* Strauss tested by an Improved Standardized Procedure. *Z. Wasser Abwasser Forsch.* 15(1), 1-6.
 - 156 Bringman, G. und Kühn, R. (1977): Results of the Damaging Effect of Water Pollutants on *Daphnia Magna*. *Z. Wasser Abwasser Forsch.* 10(5), 161-166.
 - 157 Bringman, G. und Kühn, R. (1980): Determination of Biological Damage from Water Pollutants to Protozoa. III. Saprozoic Flagellates. *Z. Wasser Abwasser Forsch.* 13(5), 170-173.
 - 158 Bringman, G. und Kühn, R. (1978): Testing of Substances for their Toxicity Threshold: Model Organisms *Microcystis (Diplocystis) aeruginosa* and *Scenedesmus quadricauda*. *Mitt. Int. Ver. Theor. Angew. Limnol.* 21, 275-284.
 - 159 (159)Bringman, G. und Kühn, R. (1980): Comparison of the Toxicity Threshold of Water Pollutants to Bacteria, Algae, and Protozoa in the Cell Multiplication Inhibition Test. *Water Res.* 14(3), 231-241.
 - 160 Bringman, G. und Kühn, R. (1978): Limiting Values for the Noxious Effects of Water Pollutants to Blue Algae (*Microcystis aeruginosa*) and Green Algae (*Scenedesmus quadricauda*) in the..., *Z. Vom Wasser* 50, 45-60.
 - 161 Bringman, G. und Kühn, R. (1977): Limiting Values for the Damaging Action of Water Pollutants to Bacteria (*Pseudomonas putida*) and Green Algae (*Scenedesmus quadricauda*) in the ..., *Z. Wasser Abwasser Forsch.* 10 (3/4), 87-98.
 - 162 Henkel-Report, unpublished, Final Report 882633, cited in IUCLID Data Set "Hexan-1-ol", compiled for "EG-AltstoffV", 1998.
 - 163 CONOCO Report (1965): Acute Oral Toxicity (LD₅₀) Study in Rats. Scientific Associates, Inc., No. 98652.
 - 164 Henkel-Report, unpublished, Archive No. 936, cited in IUCLID Data Set "Octan-1-ol", compiled for "EG-AltstoffV", 1994.
 - 165 Opdyke, D.L.J. (1973): *Fd. Cosmet. Toxicol.* 11, 95-115.
 - 166 CONOCO Report (1976): Acute Dermal Toxicity (LD₅₀) in Rabbits. Scientific Associates, Inc., No. 211154.
 - 167 CONOCO Report (1975): Dermal Irritation Test in Rabbits. Scientific Associates, Inc., No. 202087.

- 168 Kaestner, W.J. (1977): J. Soc. Cosmet. Chem. 28, 741-754.
- 169 CONOCO Report (1975): Eye Irritation Test in Rabbits. Scientific Associates, Inc., No. 202087.
- 170 Jacobs, G.A., Martens, M.A. (1989): Fd. Chem. Toxic. 27(4), 255-258.
- 171 Nelson, B.K. et al. (1990): Developmental Toxicology Assessment of 1-Octanol, 1-Nonanol, and 1-Decanol Administered by Inhalation to Rats. J. Am. Coll. Toxicol. 9(1), 93-97.
- 172 Henkel-Report, unpublished, Archive No. 294, cited in IUCLID Data Set"Octan-1-ol", compiled for"EG-AltstoffV", 1994.
- 173 Henkel-Report, unpublished, Registry No. 6369, cited in IUCLID Data Set"Octan-1-ol", compiled for"EG-AltstoffV", 1994.
- 174 Henkel-Report, unpublished, Registry No. 6369, cited in IUCLID Data Set"Octan-1-ol", compiled for"EG-AltstoffV", 1994.
- 175 Vaishnav, D.D. et al. (1987): Chemosphere 16, 695-703.
- 176 Henkel-Report, unpublished, Report No.RE 920219, cited in IUCLID Data Set"Octan-1-ol", compiled for"EG-AltstoffV", 1994.
- 177 Broderius, S., Kahl, M. (1985): Aquat. Toxicol. 6, 307-322.
- 178 Veith, G.D. et al. (1983): Can. J. Fish. Aquat. Science 40, 743-748.
- 179 Geiger, D.L. et al. (1985): Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*), Vol. II, Center for Lake Superior Environmental Studies, University of Wisconsin.
- 180 Linden, E. et al. (1979): Chemosphere 11/12, 843-851.
- 181 Henkel-Report, unpublished, Registry No. 7199, cited in IUCLID Data Set"Octan-1-ol", compiled for"EG-AltstoffV", 1994.
- 182 Juhnke I., Luedemann, D. (1978): Z. Wasser Abwasser Forsch. 11, 161-164.
- 183 Kühn, R. et al. (1989): Water Res. 23, 501-510.
- 184 Elliott, J.R., McElwee, A.A. (1988): Br. J. Anaesth. 60, 817-824.
- 185 Bengtsson, B.-E. und Tarkpea, M. (1983): Marine Poll. Bull. 14, 213-214.
- 186 Kühn, R. et al. (1989): Water Res. 23, 501-510.
- 187 Bringmann, G. (1975): Gesund.-Ing. 96, 238-241.
- 188 Bringmann, G. und Kühn, R. (1980): Water Res. 14, 231-241.
- 189 Kühn, R. und Pattard, M. (1990): Water Res. 24, 31-38.
- 190 Tnag, N.H. et al. (1990): J. Environ.Eng. 116, 1076-1084.
- 191 Henkel-Report, unpublished, Registry No. 7199, cited in IUCLID Data Set"Octan-1-ol", compiled for"EG-AltstoffV", 1994.
- 192 Henkel-Report, unpublished, Archive No. 281, cited in IUCLID Data Set"Decan-1-ol", compiled for"EG-AltstoffV", 1994.
- 193 Baer, F. und Griepentrog, F. (1967): F. Medizin Ernaehr. 8, 144.
- 194 CONOCO Report (1977): Prüfung der akuten Toxizität von Alfol 10 an Sprague Dawley Ratten bei oraler Verabreichung, LPT, Hamburg, 6. Mai 1977.
- 195 CONOCO Report (1965): Acute Oral Toxicity (LD₅₀) Study in Rats. Scientific Associates, Inc., No. 98653.

- 196 CONOCO Report (1976): Acute Dermal Toxicity (LD₅₀) Study in Rabbits. Scientific Associates, Inc., No. 211155.
- 197 *Fd. Cosmet. Toxicol.* 1973): 11, p 95, cited in Registry of Toxic Effects of Chemical Substances (RTECS).
- 198 CONOCO Report (1975): Dermal Irritation Test in Rabbits. Scientific Associates, Inc., No. 202088.
- 199 *Am. Ind. Hyg. Assoc. J.* (1973): 34, p 493; cited in Registry of Toxic Effects of Chemical Substances (RTECS).
- 200 *Cutaneous Toxic.* (1977): 127, p 77; cited in Registry of Toxic Effects of Chemical Substances (RTECS).
- 201 CONOCO Report (1977): Eye Irritation Test in Rabbits. Scientific Associates, Inc., No. 231768.
- 202 Opdyke, D.L. (1973): *Fd. Cosmet. Toxicol.* 11 (1), p 105.
- 203 Nelson, B.K. et al. (1990): Developmental Toxicology Assessment of 1-Octanol, 1-Nonanol, and 1-Decanol Administered by Inhalation to Rats. *J. Am. Coll. Toxicol.* 9(1), 93-97.
- 204 Henkel-Report, unpublished, Registry No. 6368, cited in IUCLID Data Set"Decan-1-ol", compiled for"EG-AltstoffV", 1994.
- 205 Vaishnav, D.D. et al. (1987): *Chemosphere* 16, 695-703.
- 206 Brooke, L.T. et al. (1984):"Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*)", Vol. I, Center for Lake Superior Environmental Studies, University of Wisconsin.
- 207 Juhnke, I. und Luedemann, D. (1978): *Z. Abwasser Forsch.* 11, 161-164.
- 208 Henkel-Report, unpublished, Report No.88-2633, cited in IUCLID Data Set"Decan-1-ol", compiled for"EG-AltstoffV", 1994.
- 209 Henkel-Report, unpublished, Registry No.7843, cited in IUCLID Data Set"Decan-1-ol", compiled for"EG-AltstoffV", 1994.
- 210 Henkel-Report, unpublished, Registry No.7200, cited in IUCLID Data Set"Decan-1-ol", compiled for"EG-AltstoffV", 1994.
- 211 Henkel-Report, unpublished, Archive No.930, cited in IUCLID Data Set"Dodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 212 CONOCO Report (1975): Acute Oral Toxicity (LD₅₀) Study in Rats. Scientific Associates, Inc., No. 98654.
- 213 *Patty's Industrial Hygiene and Toxicology*, 2nd ed., (1963) II, 1467.
- 214 CONOCO Report (1975): Dermal Irritation Test in Rabbits. Scientific Associates, Inc., No. 202091.
- 215 CONOCO Report (1975): Eye Irritation Test in Rabbits. Scientific Associates, Inc., No. 202091.
- 216 Henkel-Report (1980), unpublished, Report No.305, cited in IUCLID Data Set"Dodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 217 The Procter & Gamble Company (1980), Test articles J0171.01 and J0172.01, Rabbit Eye Irritation, 191-566, cited in IUCLID Data Set"Dodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 218 Henkel-Report (1982), unpublished, Archive No. 295, cited in IUCLID Data Set"Dodecan-1-ol", compiled for"EG-AltstoffV", 1994.

- 219 Shimizu, H. et al. (1985): Jpn. J. Ind. Health 27, 400-419.
- 220 Henkel-Report (1992), unpublished, Report No. RE 92162, cited in IUCLID Data Set"Dodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 221 Hansen, E. (1992):"Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test on 1-Dodecanol in Rats", Institute of Toxicology, Danish National Food Agency, IT 9211105.
- 222 Henkel-Report (1992), unpublished, Report No. RE 920247, cited in IUCLID Data Set"Dodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 223 Henkel-Report (1992), unpublished, Report No. RE 920025, cited in IUCLID Data Set"Dodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 224 CONDEA Vista Untersuchung, unpublished.
- 225 Babeu, L. und Vaishnav, D.D. (1987): J. Ind. Microbiol. 2, 107-115.
- 226 Dore, M. et al. (1975): La tribune de cebedeau 28, 3-11.
- 227 Gerhold, R.M. und Malaney, G.W. (1966): J. Water Pollut. Control Fed. 38, 562-579.
- 228 Williams, J.P. et al. (1966): Appl. Microbiol. 14, 156-160.
- 229 CONDEA Chemie GmbH (1997), unpublished, 1-Dodecanol, Fish, Acute Toxicity, Henkel KgaA, TTB-Ecology, Final Report No. R 9700384.
- 230 Henkel-Report (1992), unpublished, Report No. RE 920019, cited in IUCLID Data Set"Dodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 231 CONDEA Chemie GmbH (1997), unpublished: Examination of 1-Dodecanol in an Acute Immobilization Test in Daphnia Magna, LPT Report No. 10762/97.
- 232 Bengtsson, B.E. und Tarkpea, M. (1983): Marine Poll. Bull. 14, 213-214.
- 233 Bengtsson, B.E. et al. (1984): Chemosphere 13, 613-622.
- 234 Henkel-Report , unpublished, Report No. RE 920095, cited in IUCLID Data Set"Dodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 235 Henkel-Report (1992), unpublished, Report No. RE 920200, cited in IUCLID Data Set"Dodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 236 CONDEA Chemie GmbH (1997), unpublished: Algal Growth Inhibition Test (Scenedesmus subspicatus) of 1-Dodecanol, LPT Report No. 10763/97.
- 237 Henkel-Report , unpublished, Report No. R 9400236, cited in IUCLID Data Set"Dodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 238 CONOCO Report (1977): Acute Oral Toxicity (LD₅₀) in Rats. Scientific Associates, Inc., No. 233620.
- 239 CONOCO Report (1977): Acute Oral Toxicity (LD₅₀) Study in Rats. Scientific Associates, Inc., No. 98655.
- 240 Food Cosmet. Toxicol. (1975), 13, 699-700.
- 241 CONOCO Report (1977): Acute Dermal Toxicity (LD₅₀) in Rabbits. Scientific Associates, Inc., No. 233620
- 242 CONOCO Report (1977): Dermal Irritation Test in Rabbits. Scientific Associates, Inc., No. 233620
- 243 Food Cosmet. Toxicol. (1975), 13, 699-700.
- 244 CONOCO Report (1977): Eye Irritation Test in Rabbits. Scientific Associates, Inc., No. 233620

- 245 Henkel-Report , unpublished, Archive No. 232, cited in IUCLID Data Set "Tetradecanol", compiled for"EG-AltstoffV", 1994
- 246 Food Cosmet. Toxicol. (1975), 13, 699-700.
- 247 Henkel-Report , unpublished, Report No. RE 920026, cited in IUCLID Data Set"Tetradecanol", compiled for"EG-AltstoffV", 1994.
- 248 CONDEA Vista (1994), unpublished: Biodegradability of eleven VISTA Alcohols, TSR-No. 6940.
- 249 CONOCO Report (1965): Acute Oral Toxicity (LD₅₀) Study in Rats. Scientific Associates, Inc., No. 98656.
- 250 Henkel-Report , unpublished, Archive No. 944, cited in IUCLID Data Set"hexadecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 251 Anonymous (1988): Final Report on the Safety Assessment of Cetearyl alcohol, Cetyl Alcohol, Isostearyl Alcohol, Myristyl Alcohol, and Behenyl Alcohol; J. Am. Coll. Toxicol., Vol. 7(3), 359-411.
- 252 Opdyke, D.L.J. (1978): Fragrance Raw Materials Monographs"Cetyl alcohol"; Food Cosmet. Toxicol. 16, 683-686.
- 253 Gloxhuber, Ch. (1983): Aertzliche Kosmetologie 13, 181-186.
- 254 Henkel-Report (1985), unpublished, Archive No. 85 0499, cited in IUCLID Data Set"hexadecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 255 CONOCO Report, unpublished (1966): Final Report on the Thirteen-Week Subacute Feeding of ALFOL 16 to Rats, Scientific Associates, Inc., Report No. 823.
- 256 CONOCO Report, unpublished (1966): Final Report on the Thirteen-Week Subacute Feeding in Beagle Dogs of ALFOL 16, Scientific Associates, Inc. Report No. 824.
- 257 Henkel-Report , unpublished, Archive No. 236, cited in IUCLID Data Set"hexadecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 258 Henkel-Report (1992), unpublished, Report No. RE 920102, cited in IUCLID Data Set"hexadecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 259 CONDEA Vista (1994), unpublished: Biodegradability of eleven VISTA Alcohols, TSR-No. 6940.
- 260 (260)MacPhee, C., Ruelle, R. (1969): Lethal Effects of 1888 chemicals upon four species of fish from western North America. Idaho For. Wildl. Range Exp. Stn. Bull. 3, 1-112.
- 261 Berger, B.B. (1958): J. Am. Water Works Assoc. 50, 855-858.
- 262 Henkel-Report (1992), unpublished, Report No. RE 920039, cited in IUCLID Data Set"hexadecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 263 CONOCO Report (1965): Acute Oral Toxicity (LD₅₀) in Rats. Scientific Associates, Inc., No. 98657.
- 264 Henkel-Report , unpublished, Archive No. 956, cited in IUCLID Data Set"octadecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 265 Burkhard, L.P., Kühl, D.W. und Veith, G.D. (1985): Chemosphere 14, 1551-1560.
- 266 Anonymous (1985):"Final Report on the Safety Assessment of Stearyl Alcohol, Oleyl Alcohol, and Octyl Dodecanol", J. Am. Coll. Toxicol. 4(5), 1-29.

- 267 Henkel-Report (1986) , unpublished, Archive No. 86 0070, cited in IUCLID Data Set"octadecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 268 Henkel-Report, unpublished, Archive No. 237, cited in IUCLID Data Set "octadecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 269 Blevins, R. et al. (1982):"Mutagenicity Screening of Twenty-Five Cosmetic Ingredients with the Salmonella/Microsome Test", J. Environ. Sci. Health, A17(2), 217-239.
- 270 Hansen, E. (1992):"Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test on 1-Dodecanol in Rats", Institute of Toxicology, Danish National Food Agency, IT 911130.
- 271 Henkel-Report (1992), unpublished, Report No. 92 0246, cited in IUCLID Data Set"octadecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 272 Henkel-Report (1992), unpublished, Report No. 92 0028, cited in IUCLID Data Set"octadecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 273 Henkel-Report (1992), unpublished, Report No. 92 0219, cited in IUCLID Data Set"octadecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 274 Henkel-Report (1993), unpublished, Report No. 93 00206, cited in IUCLID Data Set"octadecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 275 Henkel-Report (1992), unpublished, Report No. 92 0020, cited in IUCLID Data Set"octadecan-1-ol", compiled for"EG-AltstoffV", 1994
- 276 Henkel-Report (1992), unpublished, Report No. 92 0096, cited in IUCLID Data Set"octadecan-1-ol", compiled for"EG-AltstoffV", 1994
- 277 Henkel-Report (1992), unpublished, Report No. 92 0040, cited in IUCLID Data Set"octadecan-1-ol", compiled for"EG-AltstoffV", 1994
- 278 Henkel-Report (1994), unpublished, Report No. 94 00049, cited in IUCLID Data Set"octadecan-1-ol", compiled for"EG-AltstoffV", 1994
- 279 Henkel-Report , unpublished, Archive No. 937, cited in IUCLID Data Set "Alcohols, C12-18", compiled for"EG-AltstoffV", 1994.
- 280 Henkel-Report (1988), unpublished, Report No. 880232, cited in IUCLID Data Set"Alcohols, C12-18", compiled for"EG-AltstoffV", 1994.
- 281 Henkel-Report (1992), unpublished, Report No. 920073, cited in IUCLID Data Set"Alcohols, C12-18", compiled for"EG-AltstoffV", 1994.
- 282 Henkel-Report (1988), unpublished, Report No. 880692, cited in IUCLID Data Set"Alcohols, C12-18", compiled for"EG-AltstoffV", 1994.
- 283 Henkel-Report , unpublished, Archive No. 297, cited in IUCLID Data Set "Alcohols, C12-18", compiled for"EG-AltstoffV", 1994.
- 284 Henkel-Report (1992), unpublished, Report No. RE 920245, cited in IUCLID Data Set"Alcohols, C12-18", compiled for"EG-AltstoffV", 1994.
- 285 Henkel-Report (1972), unpublished, Archive No. 72 0089, cited in IUCLID Data Set"Alcohols, C16-18", compiled for"EG-AltstoffV", 1994.
- 286 Gloxhuber, Ch. (1983): Aertzliche Kosmetologie 13, 181-186.
- 287 Henkel-Report, unpublished, Registry No. 6603, cited in IUCLID Data Set "Alcohols, C16-18", compiled for"EG-AltstoffV", 1994.
- 288 CONDEA Chemie GmbH (1987), unpublished: Akute Toxizität- oral-NACOL 20 an Ratten, LPT Report v. 15. Januar 1987.

- 289 CONDEA Chemie GmbH (1986), unpublished: Prüfung der akuten lokalen Verträglichkeit von NACOL 20 an der Kaninchenhaut, LPT Report v. 17. November 1986.
- 290 CONDEA Chemie GmbH (1986), unpublished: Schleimhautverträglichkeit von NACOL 20 bei einmaliger Applikation in den Konjunktivalsack des Kaninchenauges, LPT Report v. 18. November 1986.
- 291 CONDEA Chemie GmbH (1987), unpublished: Akute Toxizität- oral-NACOL 22 RD an Ratten, LPT Report v. 15. Januar 1987.
- 292 CONDEA Chemie GmbH (1986), unpublished: Prüfung der akuten lokalen Verträglichkeit von NACOL 22 RD an der Kaninchenhaut (Patch-Test), LPT Report v. 17. November 1986.
- 293 CONDEA Chemie GmbH (1986), unpublished: Schleimhautverträglichkeit von NACOL 22 RD bei einmaliger Applikation in den Konjunktivalsack des Kaninchenauges, LPT Report v. 18. November 1986.
- 294 CONDEA Chemie GmbH (1986), unpublished: Akute Toxizität- oral-ISOFOL 12 an Ratten. LPT Report v. 30. Dezember 1986.
- 295 CONDEA Chemie GmbH (1986), unpublished: Prüfung der akuten lokalen Hautverträglichkeit von ISOFOL 12 an der Kaninchenhaut (Patch-Test). LPT Report v. 24. November 1986.
- 296 CONDEA Chemie GmbH (1986), unpublished: Schleimhautverträglichkeit von ISOFOL 12 bei einmaliger Applikation in den Konjunktivalsack des Kaninchenauges. LPT Report v. 13. Oktober 1986.
- 297 CONDEA Chemie GmbH (1989), unpublished: Hautverträglichkeit von ISOFOL-Alkoholen im Epicutan-Test an freiwilligen Probanden; Gutachten Prof. Dr. med. Tronnier, Hautklinik der Städtischen Kliniken Dortmund.
- 298 CONDEA Chemie GmbH (1995), unpublished: Biodegradability (21d) according to CEC L-33-T-82, Test Substance ISOFOL 12, Project No.: 950006377.372, TÜV No. C1-02/95-01.
- 299 CONDEA Chemie GmbH (1975), unpublished: Akute orale Toxizität von 2-Hexyl-decanol an Ratten bei peroraler Verabreichung., LPT Report v. 12. März 1975.
- 300 Henkel-Report , unpublished, Archive No. 700074, cited in IUCLID Data Set"2-hexal-1-decanol", compiled for"EG-AltstoffV", 1995.
- 301 CONDEA Chemie GmbH (1975), unpublished: Über die akute Toxizität von 2-Hexyl-decanol bei lokaler Applikation an Kaninchen, LPT Report v. 14. Februar 1975.
- 302 Kluge, A., Kruse, D. (1971): Eigenschaften und Verwendung eines neuen C16-Alkohols, Seifen-Öle-Fette-Wachse, Nr. 22, 827-830.
- 303 CONDEA Chemie GmbH (1989), unpublished: Hautverträglichkeit von ISOFOL-Alkoholen im Epicutan-Test an freiwilligen Probanden; Gutachten Prof. Dr. med. Tronnier, Hautklinik der Städtischen Kliniken Dortmund.
- 304 CONDEA Chemie GmbH (1975), unpublished: Schleimhautverträglichkeit von 2-Hexyl-decanol am Kaninchenauge, LPT Report v. 11. Februar 1975.
- 305 Henkel-Report , unpublished, Archive No. 700074, cited in IUCLID Data Set"2-hexal-1-decanol", compiled for"EG-AltstoffV", 1995.
- 306 Henkel-Report (1990), unpublished, Archive No. TBD 900309, cited in IUCLID Data Set"2-hexal-1-decanol", compiled for"EG-AltstoffV", 1995.

- 307 Henkel-Report (1991), unpublished, Archive No. RE 910073, cited in IUCLID Data Set"2-hexal-1-decanol", compiled for"EG-AltstoffV", 1995.
- 308 Henkel-Report , unpublished, Archive No. 8256/223-1, cited in IUCLID Data Set"2-hexal-1-decanol", compiled for"EG-AltstoffV", 1995.
- 309 CONDEA Chemie GmbH (1995), unpublished: Biodegradability (21d) according to CEC L-33-T-82, Test Substance ISOFOL 16, Project No.: 950006377.372.
- 310 Henkel-Report , unpublished, Archive No. 6803, cited in IUCLID Data Set"2-hexal-1-decanol", compiled for"EG-AltstoffV", 1995.
- 311 CONDEA Chemie GmbH (1986), unpublished: Akute Toxizität - oral-ISOFOL 18 an Ratten, LPT Report v. 27. November 1986.
- 312 CONDEA Chemie GmbH (1986), unpublished: Prüfung der akuten lokalen Verträglichkeit von ISOFOL 18 an der Kaninchenhaut (Patch-Test). LPT Report v. 26. November 1986.
- 313 CONDEA Chemie GmbH (1986), unpublished: Schleimhautverträglichkeit von ISOFOL 18 bei einmaliger Applikation in den Konjunktivalsack des Kaninchenauges. LPT Report v. 13. Oktober 1986.
- 314 CONDEA Chemie GmbH (1989), unpublished: Hautverträglichkeit von ISOFOL-Alkoholen im Epicutan-Test an freiwilligen Probanden; Gutachten Prof. Dr. med. Tronnier, Hautklinik der Städtischen Kliniken Dortmund.
- 315 CONDEA Chemie GmbH (1975), unpublished: Akute Toxizität von 2-Octyl-dedecanol an Ratten bei peroraler Verabreichung, LPT Report v. 12. März 1975.
- 316 Henkel-Report , unpublished, Archive No. 70 0015, cited in IUCLID Data Set"2-Octyldodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 317 CONDEA Chemie GmbH (1975), unpublished: Über die akute Toxizität von 2-Octyl-dedecanol bei lokaler Applikation an Kaninchen, LPT Report v. 14. Februar 1975.
- 318 Henkel-Report , unpublished, Archive No. 70 0015, cited in IUCLID Data Set"2-Octyldodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 319 Henkel-Report (1987): unpublished, Archive No. 87 0570, cited in IUCLID Data Set"2-Octyldodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 320 CONDEA Chemie GmbH (1975), unpublished: Schleimhautverträglichkeit von 2-Octyl-dedecanol am Kaninchenaugenauge, LPT Report v. 11. Februar 1975.
- 321 Henkel-Report (1989): unpublished, Archive No. 89 0350, cited in IUCLID Data Set"2-Octyldodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 322 CONDEA Chemie GmbH (1989), unpublished: Hautverträglichkeit von ISOFOL-Alkoholen im Epicutan-Test an freiwilligen Probanden; Gutachten Prof. Dr. med. Tronnier, Hautklinik der Städtischen Kliniken Dortmund.
- 323 Henkel-Report (1973): unpublished, Archive No. 73 0054, cited in IUCLID Data Set"2-Octyldodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 324 Henkel-Report, unpublished, Archive No. 58, cited in IUCLID Data Set"2-Octyldodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 325 Henkel-Report (1992), unpublished, Archive No. RT 920405, cited in IUCLID Data Set"2-Octyldodecan-1-ol", compiled for"EG-AltstoffV", 1994.
- 326 Henkel-Report, unpublished, Registry No. 6804, cited in IUCLID Data Set"2-Octyldodecan-1-ol", compiled for"EG-AltstoffV", 1994.

- 327 Henkel-Report, unpublished, cited in IUCLID Data Set "2-Octyldodecan-1-ol", compiled for "EG-AltstoffV", 1994.
- 328 Henkel-Report, unpublished, Archive No. /BIAS-No./Test-No. 9800326 2, cited in IUCLID Data Set "2-Octyldodecan-1-ol", compiled for "EG-AltstoffV", 1994.
- 329 Henkel-Report, unpublished, Archive No. /BIAS-No./Test-No. 9800326 4, cited in IUCLID Data Set "2-Octyldodecan-1-ol", compiled for "EG-AltstoffV", 1994.
- 330 CONDEA Chemie GmbH (1995), unpublished: Biodegradability (21d) according to CEC L-33-T-82, Test Article ISOFOL 20, Project No.: 950006377.372, TÜV No. C1-02/95-03.
- 331 Henkel-Report, unpublished, Registry No. 7331, cited in IUCLID Data Set "2-Octyldodecan-1-ol", compiled for "EG-AltstoffV", 1994.
- 332 Henkel-Report (1993): unpublished, Prüf-Nr.. 9300287-13, cited in IUCLID Data Set "2-Octyldodecan-1-ol", compiled for "EG-AltstoffV", 1994.
- 333 Henkel-Report, unpublished, Registry No. 7331, cited in IUCLID Data Set "2-Octyldodecan-1-ol", compiled for "EG-AltstoffV", 1994.
- 334 CONDEA Chemie GmbH (1986), unpublished: Akute Toxizität - oral-ISOFOL 24 an Ratten, LPT Report v. 27. November 1986.
- 335 CONDEA Chemie GmbH (1986), unpublished: Prüfung der akuten lokalen Verträglichkeit von ISOFOL 24 an der Kaninchenhaut (Patch-Test). LPT Report v. 26. November 1986.
- 336 CONDEA Chemie GmbH (1986), unpublished: Schleimhautverträglichkeit von ISOFOL 24 bei einmaliger Applikation in den Konjunktivalsack des Kaninchenauges. LPT Report v. 13. Oktober 1986.
- 337 CONDEA Chemie GmbH (1989), unpublished: Hautverträglichkeit von ISOFOL-Alkoholen im Epicutan-Test an freiwilligen Probanden; Gutachten Prof. Dr. med. Tronnier, Hautklinik der Städtischen Kliniken Dortmund.
- 338 CONDEA Chemie GmbH (1995), unpublished: Biodegradability (21d) according to CEC L-33-T-82, Test Substance ISOFOL 24, Project No.: 950006377.372, TÜV No. C1-02/95-04.

Copyright © 2000 by CONDEA

Fatty alcohols and derivatives

Summary

CONDEA has the most diversified portfolio of linear fatty alcohols between C4 and C22+. As the leading supplier of fatty alcohols to the chemical industry, there are many applications for a wide variety of products, including metalworking compounds, flavors and fragrances, personal care products, cosmetics, plastic additives, detergents and cleaners. CONDEA also uses fatty alcohols in its own operations to make surfactants that serve as detergent raw materials and to make specialty plasticizers.

Fatty alcohols from CONDEA meet the highest environmental standards. Their chemical structure makes

them non-toxic and completely biodegradable. And as they are easily converted into derivatives, fatty alcohols are in great demand as intermediates.

One of CONDEA's particular strengths lies in the unique capabilities of its manufacturing facilities. They produce linear and semi-linear fatty alcohols from petrochemical feedstocks and oleochemical raw materials. CONDEA enhances its alcohol product portfolio by also producing mono branched oxo alcohols as well as defined mono branched Guerbet alcohols.

This combination of manufacturing processes provides a high degree of flexibility and helps us to meet the customers' demand for tailor-made products. Most ALFOL alcohols are virtually interchangeable with corresponding NACOL, NAFOL and LINCOL products. This allows CONDEA to ship from the most favourable logistics location to our global customers.

Production sites:

Augusta (Italy)
Brunsbüttel and Marl (Germany)
Lake Charles (Louisiana, US)

For more information, please e-mail to: fatty.alcohols@condea.de