Shell

NEODOL® Alcohols and Ethoxylates

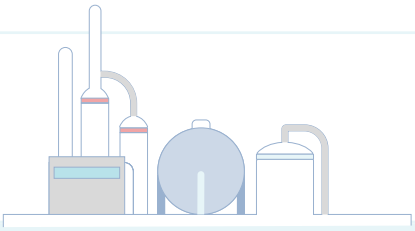
First choice for flexibility and performance

Why buy from Shell?

Shell NEODOL® alcohols and ethoxylates are used by leading manufacturers of many different consumer and industrial products, ranging from laundry and dishwashing liquids to oilfield chemicals, from hard surface cleaners to lubricants.

Within the range of C9 to C15 alcohols, we offer a wide variety of unique alcohols and ethoxylates containing the blends of carbon chains needed to match your requirements.

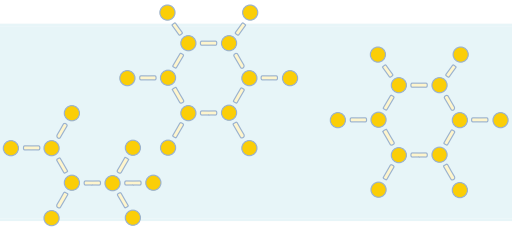
We have deep
EXPERIENCE
as a supplier, with over 80 years of expertise and performance.



Our brand stands for
QUALITY
We offer global Quality Assurance as well as Product & Technical support through our world class Technology Centres in Amsterdam and Houston.

We ensure that our substances
COMPLY
with regional and national product safety regulations.

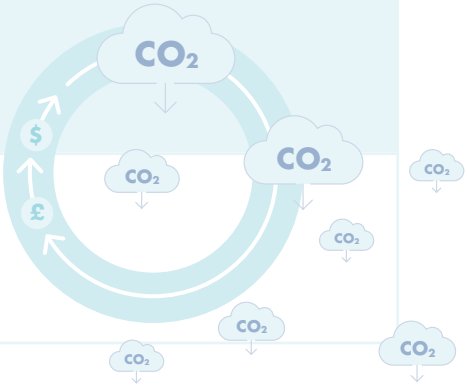
Our proprietary Shell Higher Olefins Process (SHOP) and Shell Hydroformylation (SHF) processes underpin the
FLEXIBILITY
of the molecules we can supply.



We have global reach and a record of
RELIABLE SUPPLY
on a large scale.

Our lightly branched alcohols and alcohol ethoxylates deliver
OPTIMISED PERFORMANCE
in terms of cleaning, solubility, biodegradability and ease of formulation.

We are developing
SUSTAINABLE PRODUCTS
and solutions that will reduce the CO_2 intensity of our products and enable the circular economy.



A more sustainable future

As part of the Shell commitment to a net-zero CO_2 emissions future and in response to growing customer demand for more sustainable products, we are developing **three distinct offers**:

Circular Solutions

We have started using feedstock made from plastic waste at our chemicals sites as part of our ambition to **process one million tonnes of plastic waste a year by 2025**. The resultant products match the performance, quality and specification of those made directly from fossil fuel feedstock. Our strategic agreement with pyrolysis technology company, BlueAlp Holding BV, will help to accelerate this journey.

Bio-based Solutions

Bio-based Solutions is our term for our portfolio of high-quality chemical products derived from processing bio-based feedstocks, **offering carbon emissions reduction without compromising on quality or performance.** These products are independently certified and audited, supporting the credibility and transparency of our manufacturing process.

Lower Carbon Solutions

Shell is developing solutions to offer lower carbon products that **maintain the same specifications and performance while generating less CO_2** through energy efficiency, lower carbon energy sources, and carbon capture and storage (CCS). This range of solutions will help reduce greenhouse emission while helping differentiate your company and products in competitive markets.

Making our Shell NEODOL® alcohols and ethoxylates products

Shell NEODOL alcohols and ethoxylates are made at the world scale manufacturing plant in **Geismar, USA** using a proprietary manufacturing process based on ethylene.

We also have an ethoxylation unit in **Singapore** and tolling capacity in **Europe**, helping ensure global supply capabilities. Our alcohols have odd and even carbon number chains with approximately 80% linearity. Light branching within the Shell NEODOL alcohols and ethoxylates alcohols occurs predominantly at the 2-alkyl position.

Shell NEODOL alcohols and ethoxylates are easy to formulate with and handle because of their branching profile combined with variation in carbon number.

Shell NEODOL alcohols and ethoxylates' differentiated performance

Shell's proprietary Hydroformylation (SHF) process yields ~80% linear and ~20% branched carbon chains.

The Shell NEODOL alcohols and ethoxylates alcohol portfolio has blends with both even and odd numbered carbon chains. The unique combination of linearity/branching and carbon chain variation provides Shell NEODOL alcohols and ethoxylates with a good balance across several key surfactant properties including pour point, dissolving time, wetting time, critical micelle concentration, foaming, viscosity and biodegradation. This translates into higher performance in a range of applications.

	Effect of branching	Benefit of light branching
Pour point	↓	Good for handling
Dissolution time	↓	Good for formulating
Wetting time	↓	Good for spreading
Critical micelle concentration	↑	Good for emulsification and cleaning
Foaming	↓	Depends on application
Viscosity	↓	Depends on application
Biodegradability	↓	Good biodegradability

Table 1: Effect of alcohol branching on key properties of Alcohol Ethoxylates and Alcohol Ethoxy Sulfates, and the net effect for Shell NEODOL alcohols and ethoxylates alcohol light branching on these properties. Green indicates advantageous impacts, amber indicates disadvantageous impacts.

As shown in Table 1, a minimum level of branching has advantages, too much can have disadvantages. The right-hand column shows the net benefit of surfactants based on 20% lightly branched Shell NEODOL alcohols and ethoxylates alcohols.

Table 2: Shell NEODOL alcohol properties

Shell NEODOL	91	1	23	25	45	3	5	135
Carbon chain	C_9 C_{10} C_{11}	C_{11}	C_{12} C_{13}	C_{12} C_{13} C_{14} C_{15}	C_{14} C_{15}	C_{13}	C_{15}	C_{11} C_{13} C_{15}
Molecular weight, g/mol	160	172	194	207	221	200	228	207
Hydroxyl number, mg KOH/g	350	325	289	271	254	281	246	271
Flash point via PMCC, °C	108	121	135	149	157	143	149	143
Pour point, °C	-12	11	15	20	29	27	38	24
Viscosity at 40°C, cSt	9	11	13	14	18	11	15	15
Density at 25°C (or at 40°C), kg/l	0.827	0.828	0.831	0.832	0.833	(0.839)	(0.842)	0.832

Table 3: Shell NEODOL alcohol ethoxylate properties

Shell NEODOL	91-5	91-6	91-8	23-2	25-3	25-7	45-7	135-1*	135-3*	135-7*
EO groups/alcohol	5.0	6.0	8.0	2.0	2.85	7.0	7.4	1.0	2.85	7.0
Active content, %w	100	100	100	100	100	100	100	100	100	100
HLB number	11.6	12.5	13.7	6.5	7.5	12.2	11.8	3.5	7.5	12.2
Molecular weight, g/mol	380	426	510	282	332	515	546	250	332	515
Hydroxyl number, mg KOH/g	148	132	110	199	169	109	103	224	169	109
Flash point via PMCC, °C	150	150	160	152	163	186	190	146	161	186
Pour point, °C	4	6	16	0	5	19	24	13	5	18
Viscosity at 40°C, cSt	18	21	27	14	17	32	35	12	17	31
Cloud point, °C	32	54	82			47	46			46
Cloud Point, ml H_2O titrated				23	31			10	32	
Water, %w	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
1,4-Dioxane, mg/kg	< 1	< 1	< 1	< 1	< 1	< 1	< 1	< 1	< 1	< 1
Density at 40°C, kg/l	0.964	0.976	0.996	0.891	0.908	0.972	0.969	0.859	0.911	0.966

*Shell NEODOL alcohols and ethoxylates 135-1, 135-3 and 135-7 are new grades for test marketing

The N135 alcohol (with C11, 13 and 15 alcohols) is designed to have the same average molecular mass and carbon number as N25 (with C12, 13, 14 and 15 alcohols). This means that the N135 alcohol and the resulting ethoxylates have similar properties to the analogous N25 grades.

What's in a name?

The first part of a Shell NEODOL alcohols and ethoxylates grade name reflects the parent alcohol. For example, Shell NEODOL alcohols and ethoxylates 23 is a blend of C12 and C13 alcohols. The number that follows indicates the average moles of Ethylene Oxide (EO) added. So, Shell NEODOL alcohols and ethoxylates 23-2 has an average of approximately 2 moles of EO per mole of alcohol.

How Shell NEODOL® alcohols and ethoxylates can help with cold water washing

A typical laundry detergent Life Cycle Assessment would show that by far the highest CO_2 contribution (>60%) occurs **during the washing stage, due to the energy and CO_2 associated with heating water**. (Source: P&G June 2021: Can washing your clothes on cold do a world of good? https://us.pg.com/blogs/pg-sustainability-tide-ariel-cold-water-wash/) Reducing the wash temperature dramatically reduces energy usage.

The "workhorse" component in a laundry detergent is the surfactant which provides the chemical energy to clean clothes. The Shell NEODOL alcohols and ethoxylates portfolio provides intermediates to surfactants. Alcohol ethoxylates with longer ethylene oxide chains (e.g. N25-7) provide end surfactants for laundry products.

The combination of structures **deriving from Shell NEODOL alcohols and ethoxylates alcohol** - branching and variation in carbon number - **helps balance colder water solubility and lower surface tension/good cleaning**.

Shell NEODOL alcohols and ethoxylates light alcohol ethoxylates

Light alcohol ethoxylates based on N91 and N1 alcohols (with C9-11 and C11 carbon numbers, respectively) are small, mobile molecules with light branching that result in low dynamic surface tension (rapid reduction in surface tension after application) and low oil/water interfacial tension.

These properties in turn give:

- **Rapid wetting on**, for example, ceramic tiles, linoleum, steel plates in consumer & Industrial and Institutional applications.
- **Fast cleaning and excellent soil removal**, for example in hard surface cleaning applications such as in the bathroom and kitchen.
- **Rapid wetting** on waxy leaf surfaces, enabling the spreading of agrochemical formulations.
- Excellent **emulsification properties** (maintaining a homogenous product formulation).
- Excellent **water solubility and compatibility with other components**, minimising the need for hydrotropes in formulations.

1,4-Dioxane in Shell NEODOL alcohols and ethoxylates

1,4-Dioxane (1,4-D) is a by-product formed at low concentration during the manufacture of the Alcohol Ethoxy Sulfate (AES) surfactant. It is also present at trace levels in Alcohol Ethoxylates. Legislation in New York state has set a 2 ppm (2 mg/kg) maximum level for 1,4-D in on-the-shelf cleaning products by the end of 2022 and 1 ppm (1 mg/kg) by the end of 2023. California and New Jersey have similar regulatory plans and 1,4-D is a substance of very high concern (SVHC) in the European Union. **Limiting the amount of 1,4-D in cleaning and other products is, therefore, desirable**.

In 2021, Shell Chemicals presented a paper titled "1,4-dioxane in Alcohol Ethoxylates: Concentration, Measurement Methods and Mechanism of Formation" at the American Oil Chemists Society (AOCS) conference. This paper showed that **under basic (KOH) ethoxylation conditions, 1,4-D formation is at trace levels**. Since the levels are so low, a highly sensitive GC/MS method with Single Ion Monitoring (SIM) has been developed by the American Cleaning Institute (ACI). Shell was part of the development of this method which gives extremely low detection and quantitation limits. Shell results with this method show that Shell NEODOL alcohols and ethoxylates have very low levels of 1,4-D. Technical data sheets for Shell NEODOL alcohols and ethoxylates report **a 1,4-D concentration of less than 1 ppm** (1 mg/kg).

Biodegradation of Shell NEODOL alcohols and ethoxylates products

All Shell NEODOL alcohols and ethoxylates grades are readily biodegradable. Shell NEODOL alcohols and ethoxylates based surfactants biodegrade rapidly and completely owing to their chemical structure which makes them **capable of being metabolised by microorganisms**. Shell has used tests following the OECD protocol to establish the biodegradability of Shell NEODOL alcohols and ethoxylates products. The Environmental Protection Agency has published guidelines for testing the primary and ultimate biodegradability of surfactants; Shell NEODOL alcohols and ethoxylates are **well within the EPA guidelines**. They are also within the comparable **European AISE guidelines**.

Advocating for sound science

As part of our Product Stewardship activities, our scientists participate as members of the following industry associations in voluntary initiatives around handling and toxicology:

- **The American Cleaning Institute** - a broad coalition of the cleaning product industry which advocates for sound science and sensible regulation.
- **CESIO (the European Committee of Organic Surfactants and their Intermediates)** – a group of manufacturers and marketers addressing specific issues relating to human health and the environment and advocating for the use of sound science in European regulations.
- **The HERA (Human & Environmental Risk Assessment) initiative** – a European partnership between the makers of household cleaning products (AISE) and the chemical industry (Cefic) which supports a risk-based approach to chemicals legislation in Europe.

To find out more about our products, visit www.shell.com/neodol

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