



OXSOFT[®]

Phthalate-free, non-VOC plasticizers
www.phthalate-free-plasticizers.com



Brief overview

In this brochure the most common and relevant plasticizer tests will be reviewed. The table below gives a brief overview of the results comparing OXSOFT plasticizers with traditional phthalate plasticizers.

OXSOFT phthalate-free, non-VOC plasticizers show best in class performance compared to traditional phthalate plasticizers

OXEA is integrated in key raw materials for this product range like 2-ethylhexanol and 2-ethylhexanoic acid, which enables OXEA to offer high standards regarding product quality, delivery performance and reliability.

Test Overview	OXSOFT DOA	OXSOFT 3G8	OXSOFT GPO	OXSOFT TOTM	DOP	DINP	DIDP
Shore A Hardness	Best in class						
100% Modulus	Best in class						
Low temperature flexibility	Very good	Best in class					
Elevated temperature volatility				Best in class			
Relative extraction resistance		Very good		Best in class			
Fogging number				Best in class		Very good	Very good
VOC data (Boiling point & GC)		Very good		Best in class			

Shore A Hardness

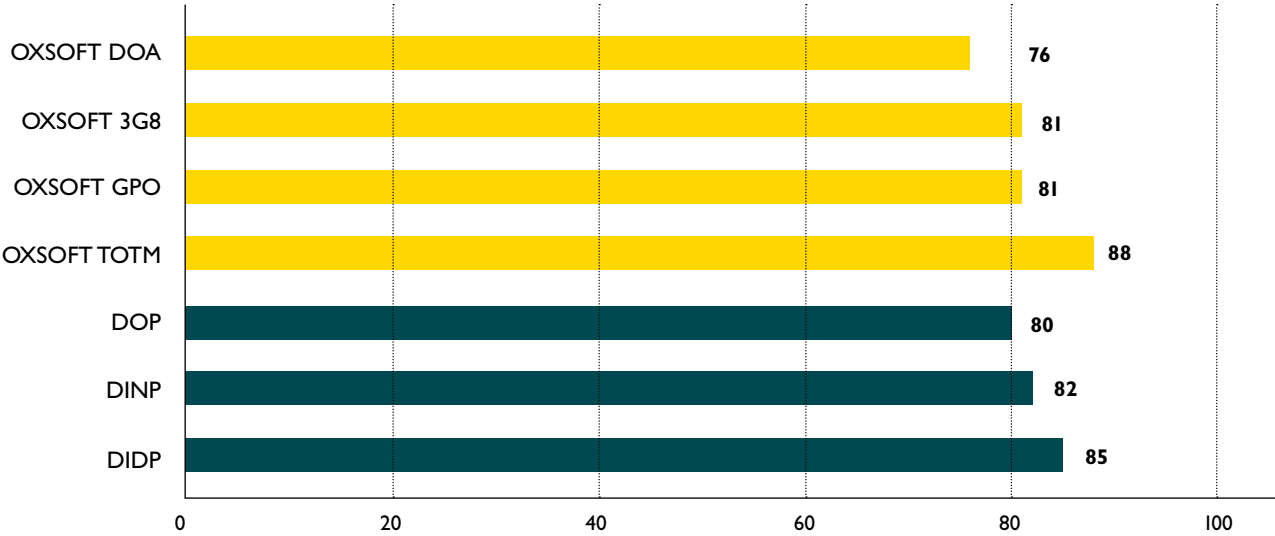
Test description

This test measures the material's ability to resist indentation under specific conditions of force and time. The preferred method for testing the relative hardness of rubbers, elastomers or softer plastics is the Shore A durometer. A Shore A durometer is a portable device that uses a truncated cone indenter point and a calibrated steel spring to measure the resistance of the elastomer to indentation.

The obtained values lie between 0 and 100. The higher the number, the greater the resistance. If the value is 0, the indenter completely penetrates the sample. If the result is 100, no penetration occurs. Shore A Hardness is an indication of the "efficiency" of the plasticizer. The lower the number the more efficient the plasticizer. Following data is based on ASTM D1706, using a plasticizer concentration in PVC of 50 phr.

Evaluation

OXSOFT DOA shows best performance and may be considered as the most efficient plasticizer. OXSOFT 3G8 and GPO show a similar performance as DOP but a slightly better performance compared to the other phthalates.



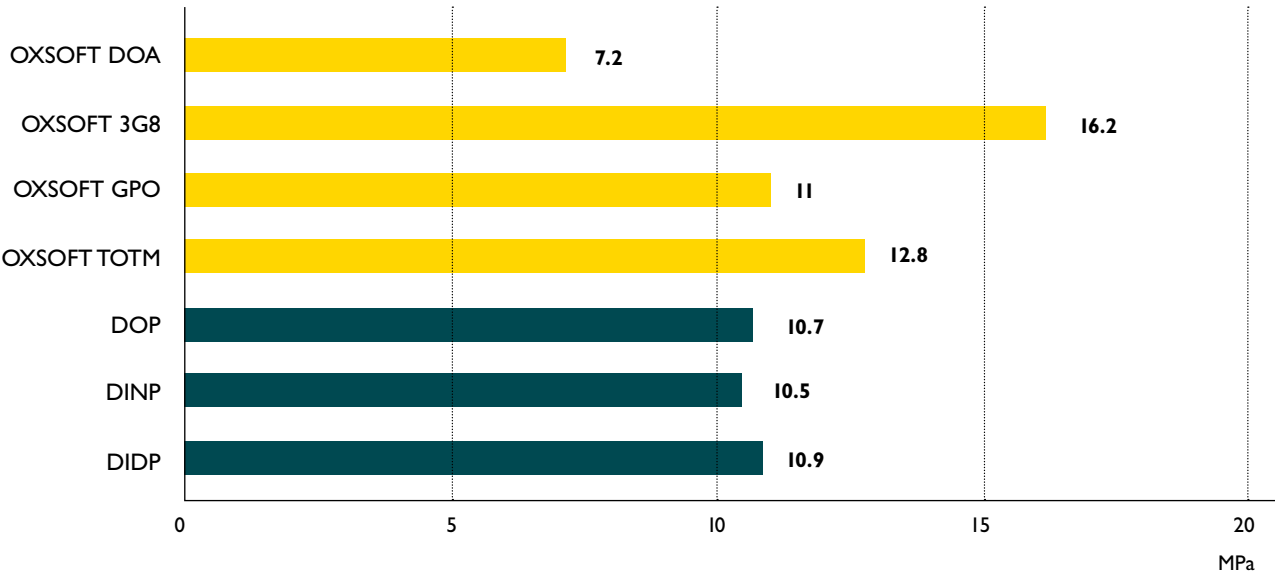
100 % Modulus

Test description

Modulus is basically the stiffness of a material, or more precisely, the force required to produce a given elongation, usually 100 per cent (100 % Modulus). Modulus is measured in MPa. Compounds with a higher modulus are more resilient and compounds with a lower modulus are more efficient. Test method is ASTM D638, using a plasticizer concentration of 50 phr in PVC.

Evaluation

OXSOFT 3G8 is by far the most resilient plasticizer, having a value of 16.2 whereas the plasticizer average of the 100% Modulus Test is around 11. OXSOFT DOA, with a relatively low value of 7.2 is obviously not as resilient as the other plasticizers, but is the most efficient one.



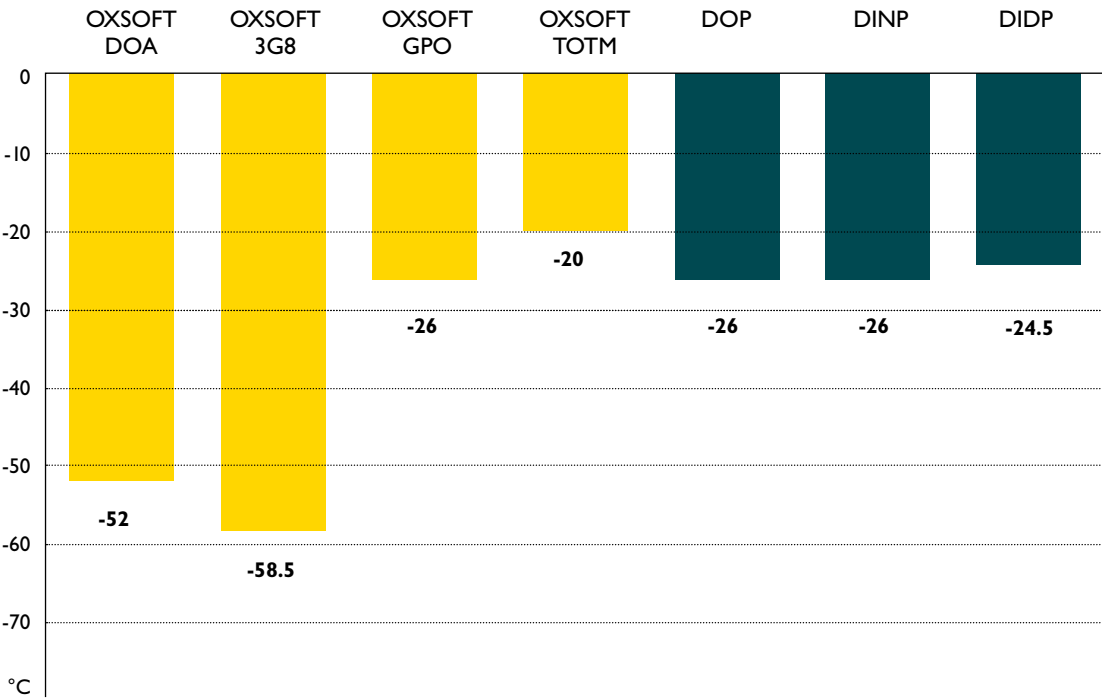
Low temperature flexibility

Test description

All plastics which are flexible at room temperature become less flexible if they are cooled, finally becoming brittle at lower temperatures. This property is often measured by torsional tests over a wide range of temperatures. The specimen is bent to an angle of 90° and examined for cracks at the bend. The temperature, where a fracture into two or more pieces, or any crack visible to the unaided eye occurs, is reported, using the test method ASTM D1043 (concentration = 50 phr).

Evaluation

OXSOFT 3G8 and DOA show by far the best low temperature flexibility. These two plasticizers are highly recommended for applications where excellent low temperature properties are required. OXSOFT GPO shows a very similar performance like traditional phthalate plasticizers.



Elevated temperature volatility

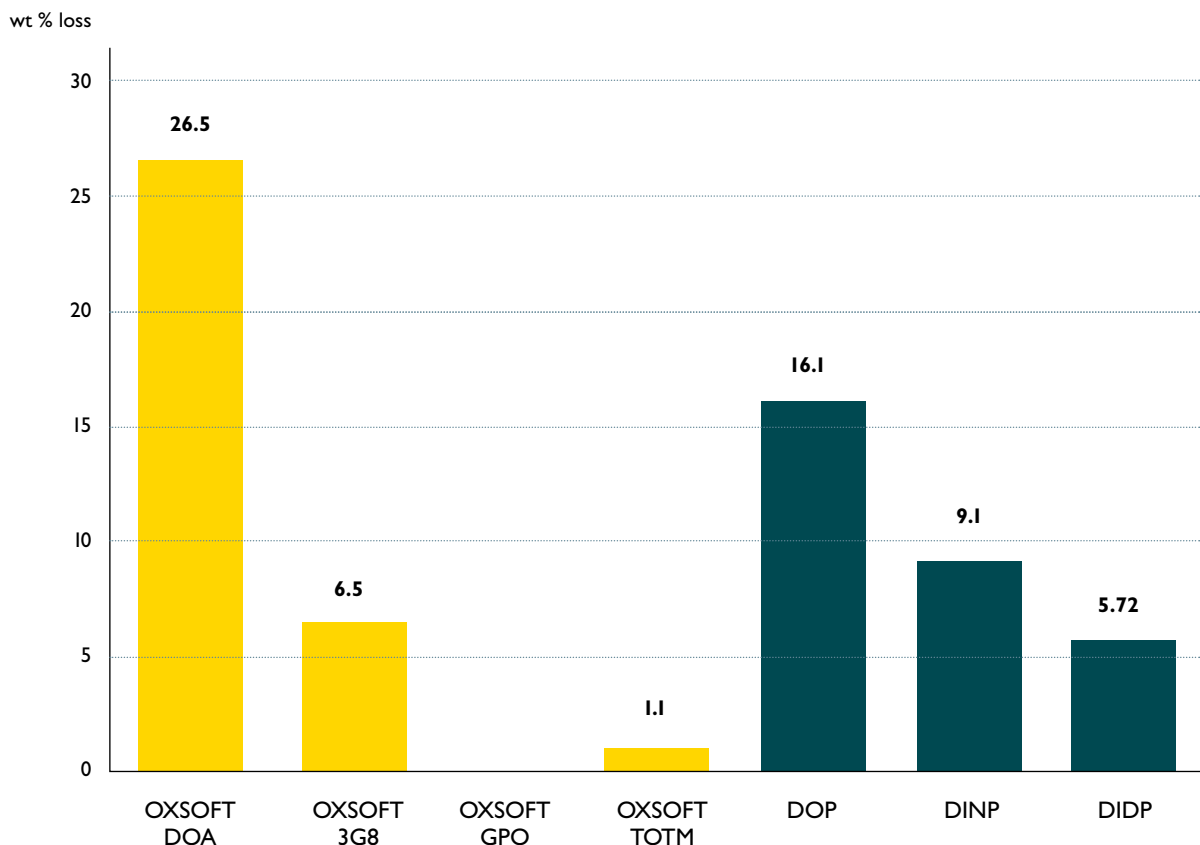
Test description

Volatility is the tendency of a substance to vaporise and is directly related to a substance's vapour pressure. At a given temperature, a substance with a higher vapour pressure vaporizes more readily than a substance with a lower vapour pressure.

Volatility is expressed as a percentage weight change (wt %) due to plasticiser loss to the atmosphere (value indicates loss of softener). Volatility loss was measured after 7 days at 100°C (concentration = 50 phr).

Evaluation

OXSOFT TOTM outperforms all included plasticizers, it offers superior permanence at elevated temperatures. OXSOFT TOTM is a highly permanent plasticizer which limits any migration concerns even at higher temperatures.



Relative extraction resistance

Test description

The relative extraction resistance intends to be a rapid empirical test to determine the loss of the plasticizer or other extractable components from the plastic film when immersed in commonly used liquids. The presented values illustrate the percentage weight change of a film after immersion in chemicals. Therefore the following three liquids were tested using the method ASTM D1239:

- Soapy water
- Oil
- Hexane

Evaluation

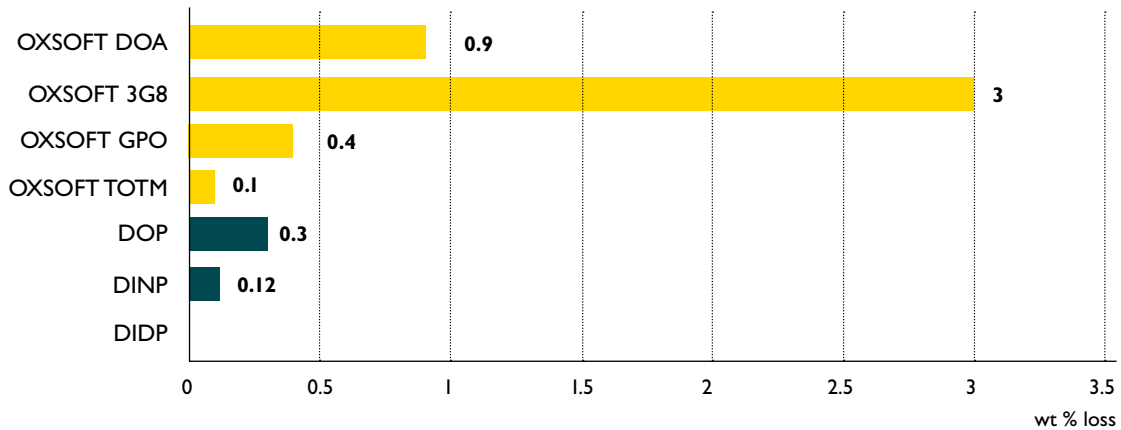
Results of plasticizer loss are very different when comparing the three liquids. With increasing wt % loss, ranking appears to be the following: soapy water < oil < hexane.

Migration of plasticizers can be a concern. For some application like medical applications any migration risk should be limited.

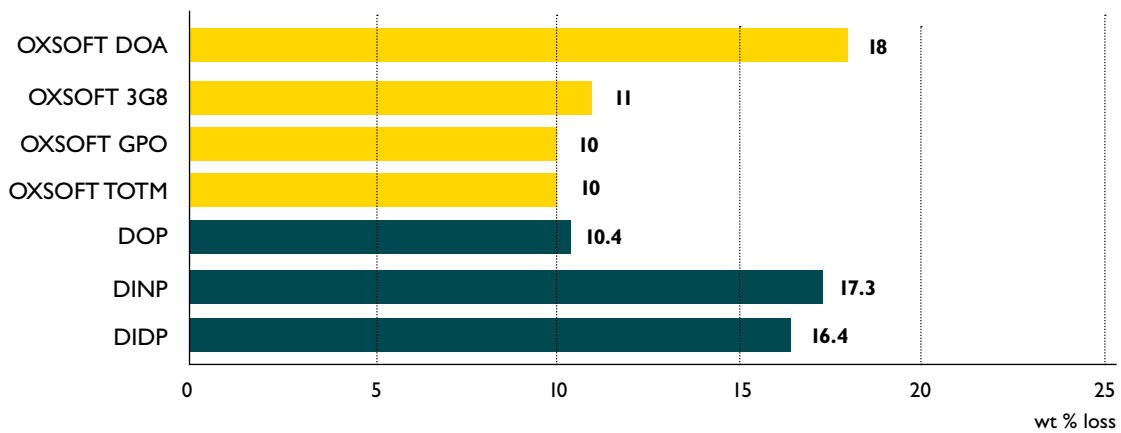
OXSOF TTM can be considered as a very permanent plasticizer. OXSOF TTM basically stays in the plastic film. OXSOF 3G8 shows good extraction resistance using oil and hexane as liquids.

Relative extraction resistance

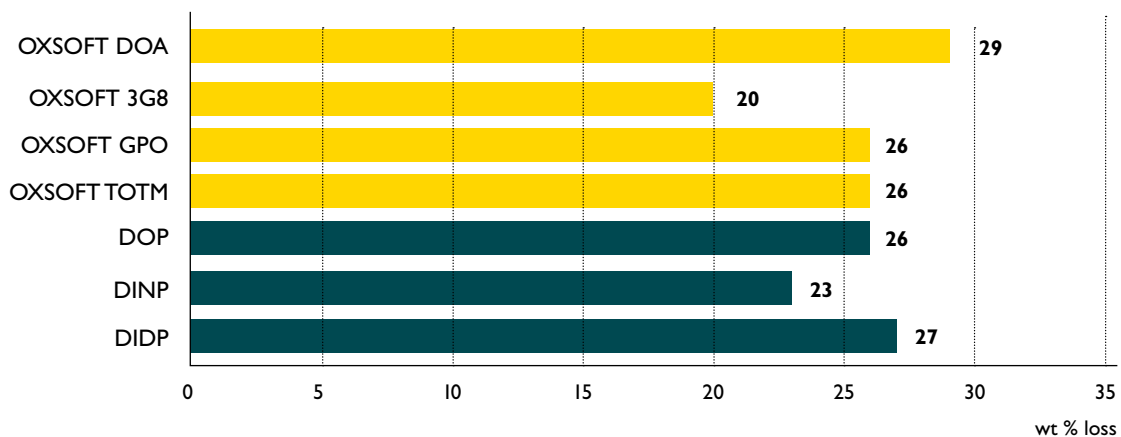
Soapy Water Extraction (ASTM D1239)



Oil Extraction (ASTM D1239)



Hexane Extraction (ASTM D1239)



Fogging number

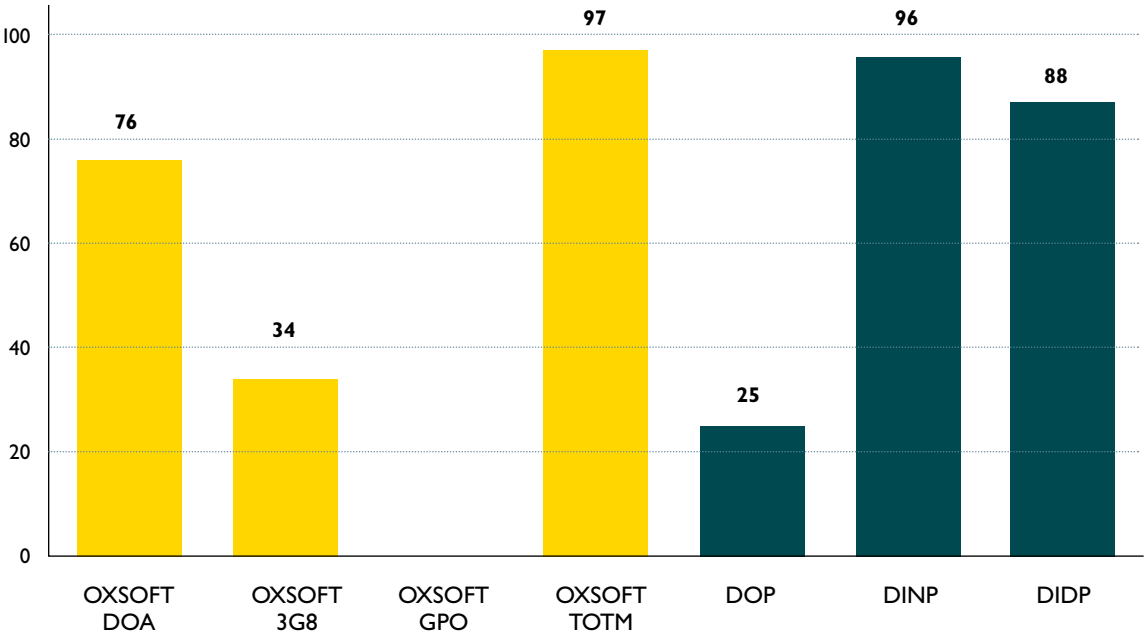
Test description

The fogging test measures the tendency for plastic or elastomeric materials to volatilize substances which can condense and collect on other surfaces when in use. It is a photometric method giving a quotient of the fogged plate and the unfogged plate multiplied by 100.

The test is used to evaluate materials to be used in automotive or other vehicle interiors. In general, automotive specifications require 1 hour fog analysis to be greater than 60. Most vinyl compounders require a minimum of 80 or better. Here, a 3 hour analysis at 100°C was applied (concentration = 67 phr).

Evaluation

OXSOFT DOA and TOTM, both having values greater than 60, meet the requirements of the automotive specifications. OXSOFT TOTM shows best in class performance.



VOC data

Test description

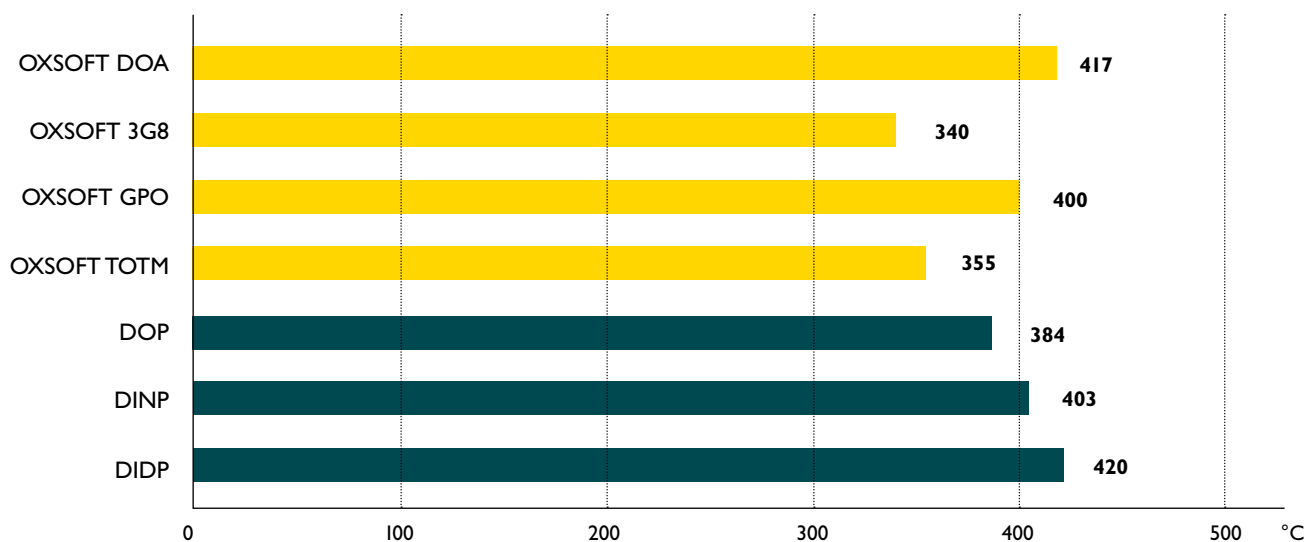
Different tests can give evidence of the volatility of the respective plasticizers. In this section, the boiling points and GC analyses are used to measure volatility.

Boiling point

In general, a compound is less volatile, the higher the boiling point. According to this statement, compounds can be divided into three different categories:

VVOC (very volatile organic compounds)	50°C–100°C
VOC (volatile organic compounds)	60°C–260°C
SVOC (semivolatile organic compounds)	over 260°C

The boiling point gives limiting information about the VOC impact of the plasticizer in the formulation. Therefore GC analysis are performed to give a better indication of the VOC impact.



VOC data – GC Analysis

Test description

The amount of VOC substances in OXSOF TTM and OXSOF 3G8 was determined by doping with n-Hexane and n-Hexadecane, since these substances are the references for classifying the examined compound into the three VOC categories (VVOC, VOC, SVOC).

Evaluation

OXSOF 3G8

OXSOF 3G8 can be classified as being only a SVOC, making it suitable for non-VOC applications. OXSOF 3G8 itself has a retention time of about 21 minutes. N-Hexadecane already elutes at the half of it after about 10 minutes.

The other recorded components n-Docosane, n-Tetracosane and n-Octacosane elute between 17 and 25 minutes – 7 to 15 minutes later than n-Hexadecane. Therefore these substances are all SVOC

OXSOF 3G8 is considered non-VOC.

OXSOF TTM

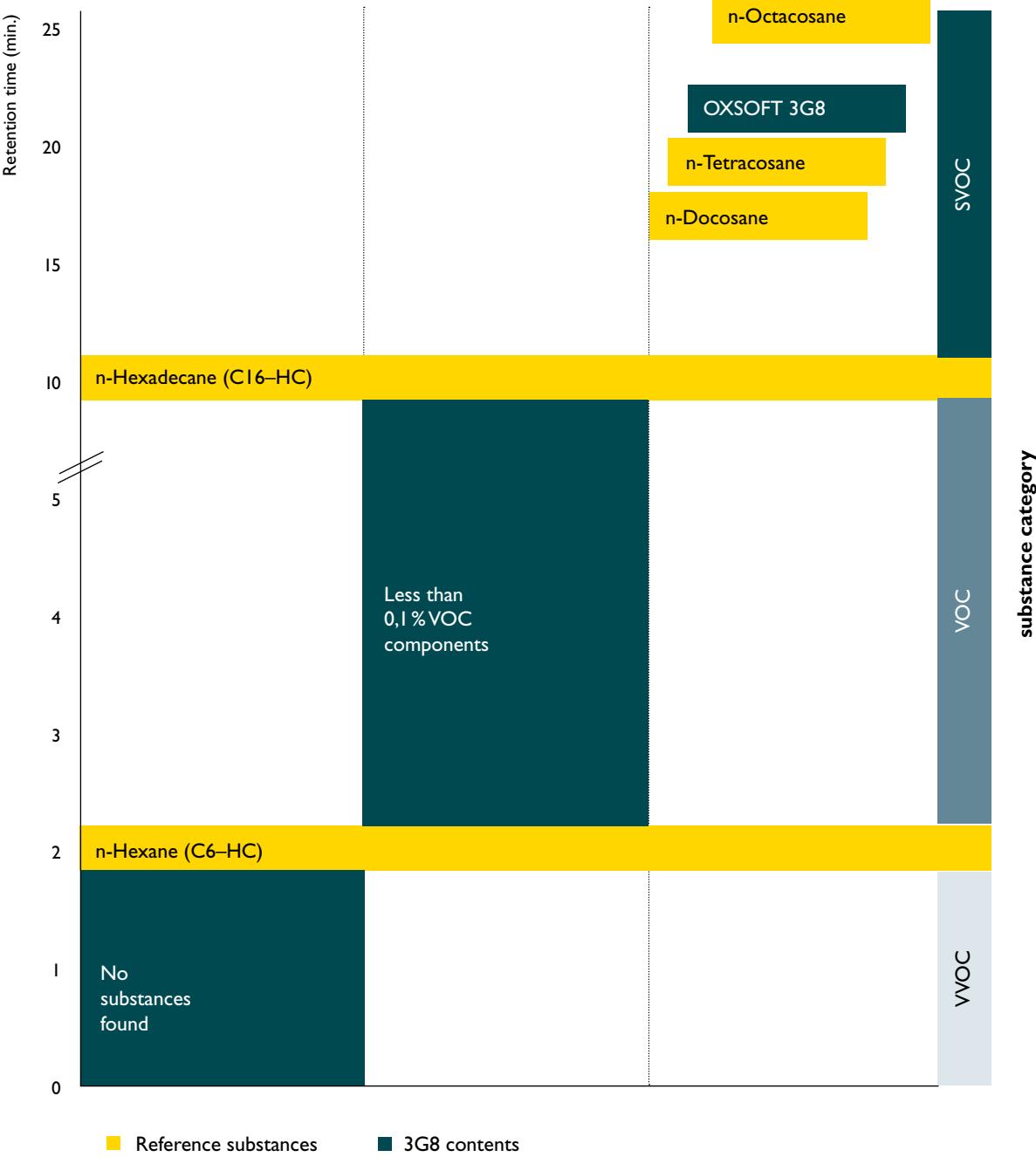
Also in this test OXSOF TTM distinguish itself being a very permanent plasticizer. It elutes after all the other reference substances and can be classified as a SVOC.

OXSOF TTM is considered non-VOC.

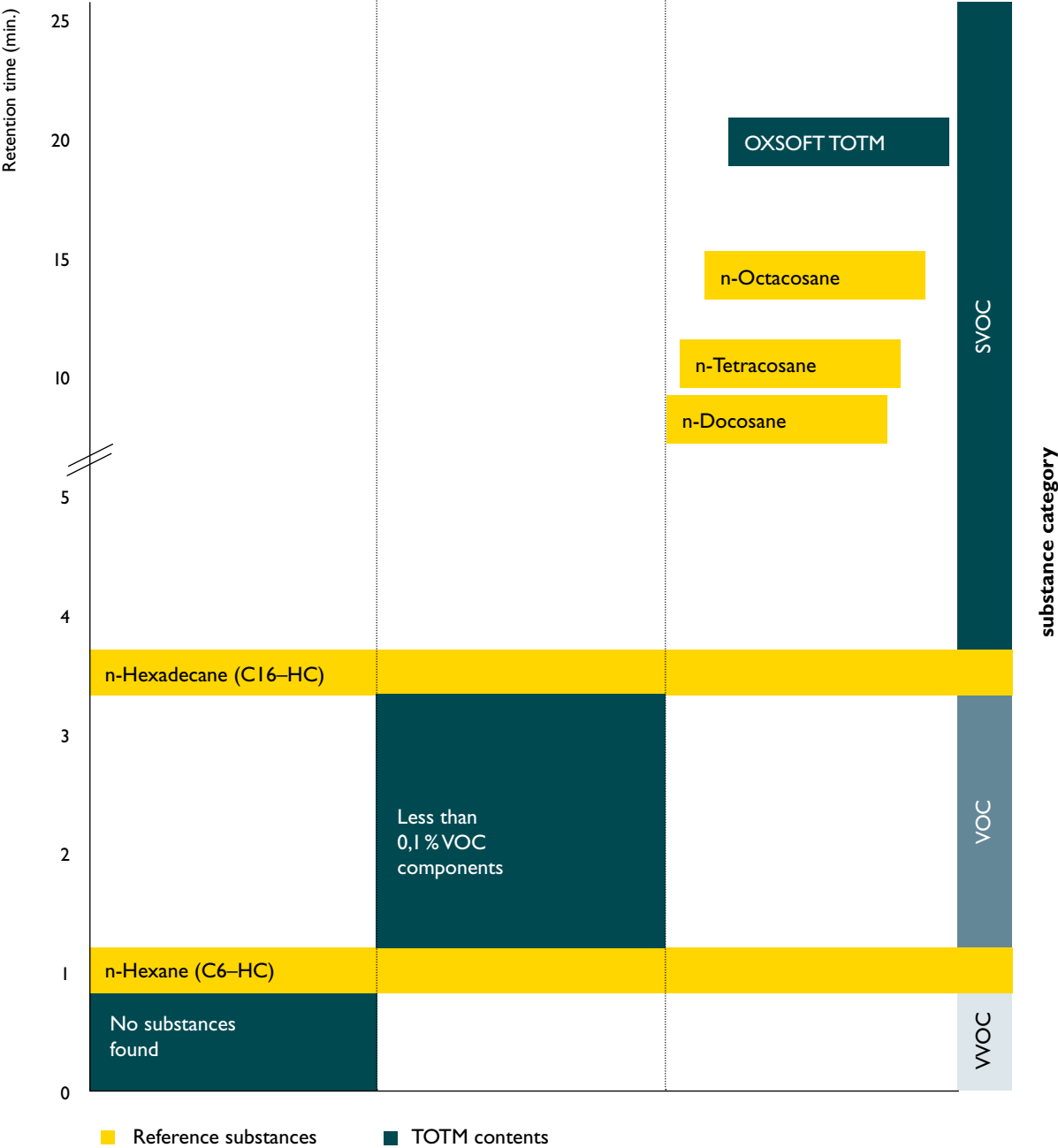
Substance classification

VVOC (very volatile organic compounds)	substances, which elute before C6-HC (n-Hexane)
VOC (volatile organic compounds)	substances, which elute between C6-HC (n-Hexane) and C16-HC (n-Hexadecane)
SVOC (semivolatile organic compounds)	substances, which elute after C16-HC (n-Hexadecane)

GC Analysis OXSOF 3G8



GC Analysis OXSOFT TOTM



Detailed Overview

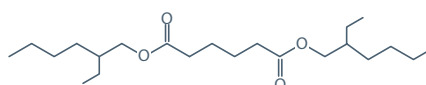
Tests and Test Method	OXSOFT DOA	OXSOFT 3G8	OXSOFT GPO	OXSOFT TOTM	DOP	DINP	DIDP
Shore A Hardness ASTM D1706, 50 phr	76	81	81	88	80	82	85
100% Modulus [mPa] ASTM D638, 50phr	7.2	16.2	11	12.8	10.7	10.5	10.9
Low temperature flexibility [°C] ASTM D1043, 50phr	-52	-58.5	-26	-20	-26	-26	-24.5
Elevated temp volatility [wt %] 100°C, 7 days, loss, 50phr	26.5	6.5		1.1	16.1	9.1	5.72
Relative extraction resistance ASTM D1239, 50phr							
soapy water extraction [wt %]	0.9	3	0.4	0.1	0.3	0.12	
oil extraction [wt %]	18	11	10	10	10.4	17.3	16.4
hexane extraction [wt %]	29	20	26	26	26	23	27
Fogging number 3 hours, 100°C, 67	76	34		97	25	96	88
VOC data (Boiling point) [°C]	417	340	400	355	384	403	420
Molecular weight (theoretical) [g/mol]	371	403	391	547	391	418	447
Specific Gravity [20/20] ASTM D4052	0.93	0.97	0.98	0.99	0.99	0.98	0.97
Refraction index (nD20) ASTM D1045	1.45	1.44	1.49	1.49	1.49	1.49	1.48
Color [APHA Pt-Co] ASTM D5386	≤ 25	≤ 30	≤ 20	≤ 30	≤ 25	≤ 25	25
Volatiles [wt %] ASTM D2369	2.41	0.53		0.14	1	0.36	
Flash point [°C] COC	196	199	238	250	218	240	232
Viscosity ASTM D445							
20°C [mm²/s]	15.1	16.3	64.1	335	86	82	121.6
40°C [mm²/s]	7.8	8.8		90		27.8	
100°C [mm²/s]	2.3	2.4	5	9.6			

OXSOFT DOA – Technical data

Application suggestion

OXSOFT DOA is a highly efficient plasticizer with excellent low temperature properties. Suggested applications are food packaging, garden hoses, gaskets, flooring and blended with other plasticizers to improve efficiency and/or low temperature properties.

CAS Number 103-23-1
EINECS Number 203-090-1



Physical and chemical properties

Formula $C_{22}H_{42}O_4$
Molecular Weight 370.6 g/mol
Appearance Clear colourless liquid
Boiling point (°C) 417
Specific Gravity (20°C) 0.925
Odour Nil
Solubility in Water (g/L, 22°C) < 0.001
Vapour pressure (hPa, 20°C) < 0.01
Viscosity (mPa*s, 20°C) 15.1

Sales Specifications

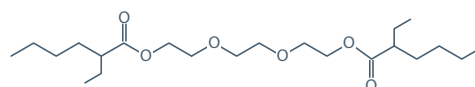
Property	Limit	Unit	Test Method	PQR
Appearance	Clear Liquid		Visual Examination	
OXSOFT DOA	min. 99.5	% (a/a)	DIN 51405 (GC)	x
Acid Value	max. 0.07	mg KOH/g	ASTM D 974 (mod.)	x
Water	max. 0.05	% (w/w)	ASTM E 1064	x
Saponification Value	298 – 306	Mg KOH/g	Calculated from GC	x
Platinum/Cobalt Colour (Hazen/APHA Colour)	max. 25		ASTM D 5386	x
Density (20°C)	0.924 – 0.926	g/cm ³	ASTM D 4052	
Refractive Index nD25	1.446 – 1.448		ASTM D 1045	

OXSOFT 3G8 – Technical data

Application suggestion

OXSOFT 3G8 combines some unique properties like superior low temperature performance, high resilience and good migration resistance. OXSOFT 3G8 shows outstanding VOC results making it suitable for all applications where non-VOC is required.

CAS Number 94-28-0
EINECS Number 202-319-2



Physical and chemical properties

Formula $C_{22}H_{42}O_6$
Molecular Weight 402.6 g/mol
Appearance Clear colourless liquid
Boiling point (°C) 340
Specific Gravity (20°C) 0.967
Odour fruity
Solubility in Water (mg/L, 20°C) 1.53
Vapour pressure (hPa, 20°C) <0.001
Viscosity (mPa*s, 20°C) 16.3

Sales Specifications

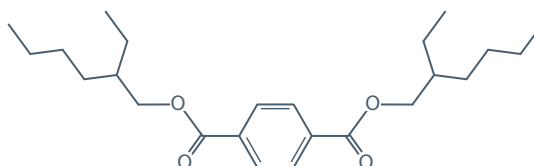
Property	Limit	Unit	Test Method	PQR
Appearance	Clear Liquid		Visual Examination	
OXSOFT 3G8	min. 97	% (a/a)	DIN 51405 (GC)	x
Triethylenglycol-mono-2-ethylhexanoate (Monoester)	max. 1.5	% (a/a)	DIN 51405 (GC)	x
Diethylenglycol-bis-2-ethylhexanoate	max. 0.5	% (a/a)	DIN 51405 (GC)	x
Acid Value	max. 0.10	mg KOH/g	DIN EN ISO 3682 / ASTM D 1613	x
Peroxide Value	max. 1.5	mäq O/kg	RCH – AL079	x
Ester Value	236 – 279	mg KOH/g	DIN 53401	
Hydroxyl Value	max. 5.0	mg KOH/g	DIN 53240	
Water	max. 0.07	% (w/w)	DIN 51777 Part I	x
BHT Stabilizer	50	mg/kg	DIN 51405 (GC), qual.	x
Platinum/Cobalt Colour (Hazen/APHA Colour)	max. 30		DIN ISO 6271	x
Density (20°C)	0.962 – 0.972	g/cm ³	DIN 51757 Verf. D	
Refractive Index nD25	1.441 – 1.447		DIN 51 423 / ASTM D 1747	

OXSOFT GPO – Technical data

Application suggestion

OXSOFT GPO is suitable as a general purpose plasticizer. The properties are very similar as DOP and OXSOFT GPO can be used as a direct replacement for DOP but also for other general purpose phthalates like DINP.

CAS Number 6422-86-2
EINECS Number 229-176-9



Physical and chemical properties

Formula $C_{24}H_{38}O_4$
Molecular Weight 390.6 g/mol
Appearance Clear colourless liquid
Boiling point (°C) 400
Specific Gravity (20°C) 0.984
Odour mild
Solubility in Water ($\mu\text{g/L}$, 20°C) negligible
Vapour pressure (hPa, 20°C) $5.56 \cdot 10^{-10}$
Viscosity (mPa*s, 25°C) 64.1

Target Sales Specifications – product launch in Q3 2011

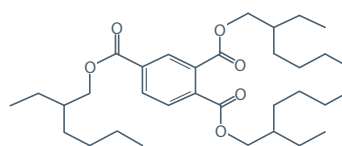
Property	Limit	Unit	Test Method	PQR
Appearance	Clear Liquid		Visual Examination	x
OXSOFT GPO	min. 96	% (w/w)	Gas Chromatography	x
Ester Content	min. 99.5	% (w/w)	Gas Chromatography	x
Free Alcohol	max. 0.01	% (w/w)	Gas Chromatography	x
Water	max. 0.05	% (w/w)	ASTM D 1364 / ASTM E 203	x
Acid Number	max. 0.05	Mg KOH/g	ASTM D 974	x
Platinum/Cobalt Colour (Hazen/APHA Colour)	max. 20		ASTM D 5386	x

OXSOFT TOTM – Technical data

Application suggestion

OXSOFT TOTM is a permanent, non-migrating plasticizer with excellent elevated temperature properties. In every application where migration is a concern OXSOFT TOTM can limit these concerns due to its permanent character. Suggested and existing applications are medical, cable and wire. In automotive and in-house applications OXSOFT TOTM is highly recommended due to outstanding fogging and non-VOC properties.

CAS Number 3319-31-1
EINECS Number 222-020-0



Physical and chemical properties

Formula $C_{33}H_{54}O_6$
Molecular Weight 546.8 g/mol
Appearance light yellow liquid
Boiling point (°C) 355
Specific Gravity (20°C) 0.986–0.990
Odour weak
Solubility in Water (g/L, 25°C) < 0.01
Vapour pressure (hPa, 20°C) < 0.001
Viscosity (mPa*s, 40°C) 90

Sales Specifications

Property	Limit	Unit	Test Method	PQR
Appearance	light Yellow Liquid		Visual Examination	
Ester Content	min. 99.0	% (w/w)	Gas Chromatography	x
OXSOFT TOTM	min. 96.0	% (w/w)	Gas Chromatography	x
GPO	max. 1.0	% (w/w)	Gas Chromatography	x
DOP	max. 0.099	% (w/w)	Gas Chromatography	x
Rest Alcohol	max. 0.1	% (w/w)	Gas Chromatography	x
Water	max. 0.1	% (w/w)	ASTM E 203	x
Acid Value	max. 0.1	mg KOH/g	ASTM D 974	x
Saponification Value	300 – 320	mg KOH/g	Calculated from GC	
Platinum/Cobalt Colour (Hazen/APHA Colour)	max. 30		ASTM D 5386	x
Cr, Ba, Pb, Cu, Sn	each < 1	mg/kg	ASTM D 5185	
Cd	< 0.6	mg/kg	ASTM D 5185	
Density (25°C)	0.986 – 0.990	g/cm ³	ASTM D 4052	
Refractive Index nD25	1.4850 – 1.4870		ASTM D 1045	

Glossary of terms

%	percentage	kg	kilogramme
% (w/w)	mass percent	KOH	Potassium hydroxide
% (a/a)	area-percent (of GC-graph)	L	liter
°C	degree Celsius	max.	maximum
3G8	Triethylenglycol-bis-2-ethylhexanoate	mg	milligram
APHA	American Public Health Association	min	minute
ASTM	American Society for Testing Materials	min.	minimum
Ba	Barium	mm ²	square millimetre
CAS	Chemical Abstracts Service	mod.	modified
Cd	Cadmium	mol	mole
cm ³	cubic centimetre	MPa	megapascal
COC	Cleveland open cup	OXSOFT	OXSOFT is a trademark of OXEA GmbH
Cr	Chromium	Pb	Lead
Cu	Copper	phr	parts per hundred of rubber
DIDP	Diisodecylphthalate	PQR	Product Quality Report
DIN	German Institute for Standardization	PVC	polyvinyl chloride
DINP	Diisononylphthalate	qual.	qualitative
DOA	Diocyladipate	s	second
DOP	Diocylphthalate	Sn	Tin
EINECS	European Inventory of Existing Commercial Chemical Substances	SVOC	semivolatile organic compounds
g	gram	TOTM	Triocyltrimellitate / Tri-(2-ethylhexyl) trimellitate
GC	Gas Chromatography	Verf.	procedure
GPO	General purpose octyl	VOC	volatile organic compounds
HC	Hydrocarbon	VVOC	very volatile organic compounds
hPa	hectopascal	wt %	percentage weight change

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OXEA is a World Leader in Oxo ...

Facts and Figures

Founded	March 1, 2007 as a buy-out from Celanese and Evonik
Owner	Advent International
Employees	approx. 1,350
Annual Sales	1.4 billion Euro
Plants	Europe: Oberhausen, Marl, Amsterdam USA: Bay City, Bishop
Offices	Europe: Oberhausen, Luxembourg Americas: Dallas, Mexico City Asia: Tokyo, Singapore, Shanghai
Products	Global supplier of Aldehydes, Oxo Alcohols, Carboxylic Acids, Polyols, Esters, Specialty Esters and Amines
Applications	Ingredients for paints & coatings, adhesives, flavors & fragrances, cosmetics, lubricants, pharmaceuticals and plastics
Sales Force	Experienced global sales team providing service to customers in Europe, the Americas and Asia
Management Team	Dr. Martina Flöel, Miguel Mantas, Cornelius Robertson and Bernhard Spetsmann
Chairman	Dr. Reinhard Gradl
Learn more about OXEA and Advent	www.oxea-chemicals.com www.adventinternational.com



OXEA

Otto-Roelen-Straße 3
46147 Oberhausen
Germany

info@oxea-chemicals.com

www.oxea-chemicals.com

www.phthalate-free-plasticizers.com