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BENZENE C_{10-13} ALKYL DERIVS

CAS-No.: 67774-74-7

EINECS-No.: 267-051-0

Summary risk assessment report

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SUMMARY RISK ASSESSMENT REPORT

Final report, 30 June 1997

Italy

Rapporteur for the risk evaluation of Benzene C_{10-13} alkyl derivs is the Ministry of Public Health, in cooperation with the Italian National Health Institute (Istituto Superiore di Sanità – ISS) which realised the scientific work for this report.

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PREFACE

This report provides a short summary with conclusions of the risk assessment report of the substance Benzene C_{10-13} alkyl derivatives that has been prepared by Italy in the context of Council Regulation (EEC) No. 793/93 on the evaluation and control of existing substances. For detailed information on the risk assessment principles and procedures followed, the underlying data and the literature references, the reader is referred to the original risk assessment report that can be obtained from the European Chemicals Bureau[1]. The present summary report should preferably not be used for citation purposes.

[1] http://ecb.ei.jrc.it

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1 GENERAL SUBSTANCE INFORMATION

Identification of the substance

CAS-No.:	67774-74-7
EINECS-No.:	267-051-0
IUPAC name:	Benzene C_{10}-$_{13}$ alkyl derivs
Synonyms:	Linear Alkylbenzene, LAB
Molecular formula:	$C_6H_5C_n\ H_{2n+1}$ n = 10 ÷13
Structural formula:	CH_3-$(CH_2)_m$-CH-$(CH_2)_n$-CH_3 (m + n = 7 - 10)
	C_6H_5
Molecular weight:	239-243
Average alkyl carbon number	C = 11.6

LAB is a mixture of C_{10}-C_{13} alkyl chain homologues with all position isomers of the aromatic ring along the linear alkyl chain, except the terminal ones.

Physico-chemical properties

Melting point:	< - 70°C
Boiling range:	278 - 314°C at 1013 hPa
Density:	0.856 - 0.866 g/cm^3
Vapour pressure at 25°C	0.013 hPa
Vapour pressure at 300°C:	3.99 hPa
Partition coefficient (log Pow):	7.5 - 9.12 at 25°C
Water solubility:	0.041 mg/l
Flash point:	140°C
Flammable limits in air:	0.45 - 10.7 vol%
Explosive properties:	none

Classification:
Classification according to Annex I of 67/548/EEC:
Not yet classified.

2 GENERAL INFORMATION ON EXPOSURE

LAB is almost entirely (> 99%) utilised as an intermediate in the production of Linear Alkylbenzene Sulphonates (LAS). Some LAB also finds minor use as solvent and binder in speciality applications, e.g. cable oil, ink industry, paint and varnishes, insulating and electricity. LAB in uses different from that of its transformation to LAS, is trivial, well below to 1% of the LAB production capacity and it can be neglected in the risk assessment. LAS is manufactured by LAB sulphonation and neutralisation of the corresponding sulphonic acid. Only a very small amount of LAB (typically 0.5%) remains in LAS as unsulphonated matter. Manufacturers use LAS in laundry detergents (granular and liquid), in some all-purpose cleaners, in some liquid dishwashing detergents, and in industrial and institutional cleaners. There are 5 production sites of LAB in Europe at the present time (1995), 3 in Italy (Augusta - Sicily, Porto Torres - Sardinia and Mantova) for a total capacity of ca. 230 kt/y, 1 in Spain (S. Roque - Cd) for a capacity of ca. 180 kt/y and 1 in Germany (Ibbenbüren) for a capacity of ca. 40 kt/y for a total production of 450 kt/y. About 230 kt/y of the European LAB production are exported world-wide. LAB is manufactured and processed in closed systems, where no emissions take place because, in addition to the low vapour pressure of LAB, all plant units are protected by pressure security valves linked to the factory blow down, in turn connected with a flare. Releases can be due mainly to tank breathing and spills at the work place. These were evaluated to be less than 1 tonne/y by an exposure profile prepared for USA LAB production. Because European LAB production is of the same order of magnitude and obtained with identical processes as those of USA, we expect equivalent amount of releases. All factory effluents are loaded to treatment plants, so that we assume a negligible entry in the aquatic system from LAB manufacturing and processing. LAB is converted to LAS in all European countries mainly by big detergent manufacturers. In the powdered detergent manufacture the low vapour pressure of LAB at 300°C suggests minimal environmental entry to the air from the spray drying treatment at this temperature. Use of improved tower scrubbers assures that this potential release is small.

3 ENVIRONMENT

3.1 EXPOSURE

The main release of LAB is in domestic sewage as unsulphonated component of LAS in detergents. We can estimate, assuming a LAS consumption in Europe of 400 kt/y, a release in the sewage for LAB of max. 2. kt/y, which are removed by biological sewage treatments plants (STPs) with an efficiency of 95-98%, with a range of 69-98% as reported in literature studies for various types of STP (including trickling filters).
General characteristics of LAB which are relevant for the exposure assessment are: no significant direct photolysis or chemical transformation, readily biodegradable, an Henry's Law constant of 95 $Pa.m^{-3}$/mol at 20°C indicating a moderate volatilisation from the water medium, measured organic carbon/water partition coefficient (Koc) of $2.2 \cdot 10^4$. From this Koc value a K_p for soil of 440 l/kg is calculated, indicating that LAB can be defined as a highly adsorptive substance.
The log Pow = 7.5 - 9.12 would predict a high potential bioaccumulation in fish but the measured BCF of 35 in a test on *Lepomis macrochirus* means a low bioconcentration.

3.1.1 PEC calculations

The exposure assessment is based on the EU-Technical Guidance Document (TGD) applying the European Union System for the Evaluation of Substances (EUSES). Monitoring data in different countries were also used. The following table summarises the local PECs derived from calculations and monitoring data for each environmental compartment.

Table 3.1 PEC values derived from local model, EUSES and monitoring.

Compartment	PEC Local Model	PEC EUSES	PEC Monitoring	PEC without STP	Unit
air (100m from STP)			3.20E-06		mg/m^3
micro-organism	0.0045				mg/l
water	0.0005	7.00E-05	0.001 TF[1] 0.0004 AS [2]	0.0075	mg/l
sediment	0.24	0.06	0.132 TF (USA) 3.16 (Japan) 0.004 (UK)	3.59	mg/kg
soil (av. time: 30 d)	0.076				mg/kg
soil (av. time: 180 d)	0.033	6.50E-04	0.026		mg/kg
ground water	8.50E-05	1.60E-06			mg/l
oral-fish	0.01				mg/kg
oral-worm	2.87				mg/kg

[1] TF: Trickling Filter
[2] AS: Activated Sludge

Estimated regional PEC values are all much lower than the concentrations near the point sources.

3.2 EFFECTS

One prolonged toxicity test on *Daphnia* is available. A 4-day algae test, covering LAB exposure over several algae generations, which can be considered as a prolonged test, is also reported.
According to TGD, if there are only two long term tests on different trophic levels but the chronic data are available for the most sensitive species, an assessment factor of 10 can be applied to the lowest NOEC. This is particularly important if the substance does not have a potential to bioaccumulate.
In the case of LAB *Daphnia* is recognised to be the most sensitive species on an acute basis and because the BCF is low it is highly probable that *Daphnia* is also the most sensitive species in chronic tests. The lowest no effect level measured in *Daphnia magna* for LAB is 0.0075 mg/l.
The extrapolation leads to a PNEC for the aquatic environment of **0.00075 mg/l.**

The PNEC for micro-organisms is extrapolated from the EC_{10} for *P. putida* (8.8 mg/l) using an extrapolation factor of 10. This leads to a PNEC of **0.88 mg/l.**

Since there are no data available for directly deriving a PNEC for the terrestrial and sediment compartment the PNEC-terrestrial and PNEC-sediment were estimated from the PNEC for aquatic organisms using the equilibrium partitioning approach. This results in a $PNEC_{terrestrial}$ of **0.29 mg/kg** and in a $PNEC_{sediment}$ of **0.32 mg/kg.**

The $PNEC_{predators}$ of **50 mg/kg** was estimated from the oral NOAEL of 50 mg/kg b.w./d.

Table 3.2 PNEC values for each environmental compartment

Compartment	PNEC	Unit
air (100m from STP)	Negligible	mg/m^3
micro-organism	10	mg/l
water	0.00075	mg/l
sediment	0.32	mg/kg
soil (av. time: 30 d)	0.29	mg/kg
soil (av. time: 180 d)	0.29	mg/kg
ground water	0.00075	mg/l
oral-fish	50	mg/kg
oral-worm	50	mg/kg

3.3 RISK CHARACTERISATION

The PEC/PNEC ratios based on the actual releases of LAB are all below 1 (**conclusion ii**).
For aquatic ecosystem using the worst monitoring data, 0.001 mg/l, a $\mathbf{PEC/PNEC_{local}}$ of **1.3** is obtained. This is, however, the worst case, because the monitoring data refer to a trickling filter (TF) STP effluent that receives no or low dilution in the receiving river. Referring to the worst LAB monitoring data of the activated sludge (AS) STP effluent, namely 0.0004 mg/l, the $\mathbf{PEC/PNEC_{local}}$ becomes equal to **0.53**, which reflects more closely the actual environmental

situation and is consistent with the calculated one. By-passing STP could lead to a $PEC/PNEC_{local}$ of 10
For sediment a **PEC/PNEC** of **0.014** is calculated using the environmental concentration (0.0044 mg/kg) coming from European monitoring, which is the worst case available value measured in UK.

The local PECs in a STP, for surface water and for soil for the various environmental exposure scenarios are presented in **Table 3.3**.

Table 3.3 PEC/PNEC ratios for micro-organisms, aquatic organisms, sediment and terrestrial organisms.

Compartment	Unit	RCR	RCR worst
air (100m from STP)	mg/m^3	<<1	
micro-organism	mg/l	0.00045	
water	mg/l	0.66667	10
sediment	mg/kg	0.75	11.22
soil (av. time: 30 d)	mg/kg	0.50345	
soil (av. time: 180 d)	mg/kg	0.11379	
ground water	mg/l	0.11333	
oral-fish	mg/kg	0.0002	
oral-worm	mg/kg	0.0574	

4 HUMAN HEALTH

4.1 EXPOSURE

The human population may be exposed to LAB at 1) the workplace, 2) from use of consumer products and 3) indirectly via the environment.

4.1.1 Workplace exposure

Because no monitoring data are available, the EASE model was used to estimate the possible exposure in workplace, both for production and transformation, assuming that no personal protective equipment (PPE) is used, including respiratory protective equipment (RPE).
Whether you assign the category of use "closed system" (with the possibility to be breached) or "non-dispersive use" to the processes, assuming that the control level is "full containment", the output of the model is the same. A process "non-dispersive use" with full containment is actually considered a "closed system". For inhalation exposure the range calculated for vapour concentration is 0-0.1 ppm (0-0.998 mg/m^3). For dermal exposure assuming that the processes are "closed system" or "non-dispersive use", a very low exposure is predicted in both cases, because no direct handling takes place. Personnel exposed to a hypothetical dermal contact can be that one involved in sampling and tank filling activity. These operations are conducted wearing PPE and last a very short period of time over the working day. In some production plants the sampling is totally automated.
In the case of plant maintenance, other personnel are involved for some hours (an average of 15 hours as a total for at least 3 workers at production plant) to cover the maintenance during the annual, or less frequent, plant shut down. Also in this operation personnel are required to wear PPE.
Considering that a direct handling occurs, with incidental contact level, a range of exposure of 0-0.1 mg/cm^2/day is predicted. Assuming that the body parts involved are hands (840 cm^2 of skin), leads to a maximum exposure of 84 mg/day (1.2 mg/kg/day assuming a body weight of 70 kg).

4.1.2 Consumer exposure

The LAB traces, present in detergents, which can come into the contact with the consumer are mainly in dishwashing by hand and hand-washing fabrics using laundry detergents.
On the basis of different assumptions, detergent manufacturers have calculated for the total dermal exposure a maximum value of $5.9 \cdot 10^{-3}$ mg/kg/day and an oral exposure of $1.9 \cdot 10^{-4}$ mg/kg/day.
The dermal exposure of $5.9 \cdot 10^{-3}$ mg/kg/day is the sum of the exposure due to hand washing of dishes and laundry; $1.9 \cdot 10^{-4}$ mg/kg/day is the oral exposure due to deposits on dishes. The latter scenario is very conservative, assuming that the uptake of the film containing residual LAB is total, without considering events such as rinsing, wiping etc.

4.1.3 Man exposed indirectly via the environment

Indirect exposure is assessed by estimating the total daily intake of a substance by consumption of food, water and inhalation of air, based on the predicted environmental concentrations in all compartments. The following table shows the total daily intakes calculated by EUSES.

Table 4.1 Summary of the indirect exposure assessment (EUSES)

Daily uptake (mg/kg body weight)		
	Model	
	Local	Regional
Air	$2.4 \cdot 10^{-6}$	$1.0 \cdot 10^{-6}$
Drinking water	$7.9 \cdot 10^{-6}$	$1.0 \cdot 10^{-6}$
Fish	$3.2 \cdot 10^{-5}$	$4.1 \cdot 10^{-6}$
Stem of plant	$3.2 \cdot 10^{-6}$	$1.6 \cdot 10^{-6}$
Root of plant	$2.5 \cdot 10^{-4}$	$7.3 \cdot 10^{-6}$
Meat	$3.5 \cdot 10^{-7}$	$1.0 \cdot 10^{-7}$
Milk	$2.07 \cdot 10^{-7}$	$6.0 \cdot 10^{-8}$
Total human dose	$\mathbf{2.5 \cdot 10^{-4}}$	$\mathbf{1.5 \cdot 10^{-5}}$

4.2 EFFECTS

LAB produces only slight acute irritation to the skin and eye of rabbits. Repeated doses give rise to inflammatory lesions of the skin of rats.
LAB is not classified as an irritant under current EU legislation.
LAB does not produce sensitisation either in experimental animals or in human volunteers. LAB is not classified as a skin sensitiser under EU legislation.
There is no evidence for an accumulation in the body by intravenous, oral and dermal route in rats. The skin contact results in only a small degree of percutaneous absorption (10% of the dose).
LAB is assumed to be rapidly and extensively eliminated principally in urine, showing only a negligible affinity to the tissues with a high lipid content or secretive actions. Moreover metabolism of the absorbed quantity is rapid and complete.
No deaths were observed in acute oral and dermal toxicity limit tests on rats (at 5000 and 2000 mg/kg respectively) and a very low inhalation toxicity was found (LC50 = 71 mg/l). LAB is not classified either toxic or harmful under current EU legislation.
Rodents exposed via inhalation to LAB for 14 weeks exhibit general eye and nose irritation, with depression of body and organ weights and elevation of liver enzymes in females only at the highest concentration tested. The NOAEL is = 0.1 mg/l.
Depressed weight gains in parental animals and in litters were observed in a two-generation reproduction study on rats at the highest dose (500 mg/kg/d).
Decreases were also found in litter size, pup viability at birth, survival and weights, however no significant effects on fertility occurred. The significant findings only at 500 mg/kg/d (for F0 and F1 adults and F1 and F2 litters) and the non-consistent effects of treatment at the lower dose, gave a NOAEL for reproductive toxicity of 50 mg/kg/d for both parental and neonatal animals.
Ossification variation and delayed ossification were found in a developmental study, however no malformations were noted.
The substance should not be considered as a developmental toxicant since an increased incidence of ossification variations and delayed ossification only at dose levels inducing maternal toxicity cannot be considered as specific effects on prenatal development. LAB does not have any unusual or selective reproductive or developmental toxicity.

LAB is both non-mutagenic and non-clastogenic, because it does not exhibit activity in test systems *in vitro* and *in vivo*.
LAB showed no skin tumourigenic or carcinogenic effects in itself and did not promote tumours induced by pre-treatment with a carcinogenic substance. However it is claimed that LAB seems to enhance the malignant lymphomas and skin tumours induced by the carcinogenic substance.
The results of this study can be misinterpreted because of high LAB concentration, resulting in hyperplastic and inflammatory lesions that is a sign that the maximum tolerable dose (MTD) has been exceeded. Several researchers have suggested that irritation and mild-long standing inflammation may enhance the carcinogenicity of small doses of a carcinogen.
In addition the investigation combined different histological type of lymphomas.
LAB was clearly not classifiable as a carcinogen according to the complete carcinogenesis study.

4.3 RISK CHARACTERISATION

4.3.1 Workplace

The low vapour pressure of LAB and the closed system processes limit exposure by inhalation. The maximum exposure predicted of 0.1 ppm (0.988 mg/m^3) can be compared with the NOAEL for inhalation of 102 mg/m^3. The margin of safety for inhalation is higher than 100 (**conclusion ii**).
The maximum dermal exposure, assuming that direct handling occurs, is predicted to be 1.2 mg/kg/d. The margin of safety can be calculated using the oral NOAEL (50 mg/kg/d) (see 4.1.2.9*) derived from reproductive toxicity data, assuming that the bioavailability for humans and the animal model and for the two exposure routes are similar. In addition the results from toxico-kinetic studies indicate that LAB is slowly absorbed through the skin, metabolised and eliminated quite completely in urine, without any accumulation. The margin of safety, in case of direct handling with incidental contact level, is calculated to be 41.6. In addition the use of proper handling procedures should avoid any possibility of exposure for workers (**conclusion ii**).

4.3.2 Consumers

The margin of safety for chronic dermal toxicity can be calculated using the oral NOAEL (50 mg/kg/d) derived from reproductive toxicity. Taking into account the consumers exposure it is possible to calculate MOSs for dermal and oral toxicity, which in the worst case are as follows:
MOS dermal = 50 / 5.9 · 10-3 = 8475
MOS oral = 50 / 1.9 · 10-4 = 263158
(**conclusion ii**).

4.3.3 Man indirectly exposed via the environment

Using again a NOAEL of 50 mg/kg/day and uptake data, namely a total human dose of $2.5 \cdot 10^{-4}$ mg/kg bw and $1.5 \cdot 10^{-5}$ mg/kg bw for local and regional models respectively, the MOS for indirectlexposure are respectively the following:
MOS Local $= 2.0 \cdot 10^5$
MOS Regional $= 3.3 \cdot 10^6$
(**conclusion ii**).

*see Benzene C10-13 Alkyl Derivs Final Report

5 RESULTS OF THE RISK ASSESSMENT

Environment

(X) ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied

Consumers

(X) ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied

Workers

(X) ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied

Indirect exposure via the environment

(X) ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied

Human health (physico-chemical properties)

(X) ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied

GLOSSARY

Standard term / Abbreviation	Explanation / Remarks and Alternative Abbreviation(s)
Ann.	Annex
AF	assessment factor
BCF	bioconcentration factor
bw	body weight / *Bw*, *b.w.*
°C	degrees Celsius (centigrade)
CAS	Chemical Abstract System
CEC	Commission of the European Communities
CEN	European Committee for Normalisation
CEPE	European Committee for Paints and Inks
d	day(s)
d.wt.	dry weight / *dw*
DG	Directorate General
DT_{50}	period required for 50 percent dissipation (define method of estimation)
DT_{50lab}	period required for 50 percent dissipation under laboratory conditions (define method of estimation)
DT_{90}	period required for 90 percent dissipation (define method of estimation)
$DT_{90field}$	period required for 90 percent dissipation under field conditions (define method of estimation)
EC	European Communities
EC	European Commission
EC_{50}	median effective concentration
EEC	European Economic Community
EINECS	European Inventory of Existing Commercial Chemical Substances
EU	European Union
EUSES	European Union System for the Evaluation of Substances
f_{oc}	organic carbon factor (compartment depending)
g	gram(s)
gw	gram weight
GLP	good laboratory practice
h	hour(s)
ha	Hectares / *h*
HPLC	high pressure liquid chromatography
IARC	International Agency for Research on Cancer
IC_{50}	median immobilisation concentration or median inhibitory concentration 1 / *explained by a footnote if necessary*
ISO	International Standards Organisation
IUPAC	International Union for Pure Applied Chemistry
kg	kilogram(s)
kPa	kilo Pascals
K_{oc}	organic carbon adsorption coefficient
K_{ow}	octanol-water partition coefficient
Kp	solid-water partitioning coefficient of suspended matter

l	litre(s) / *L*
log	*logarithm to the basis 10*
$L(E)C_{50}$	lethal concentration, median
m	meter
µg	microgram(s)
mg	milligram(s)
MOS	margins of safety
NOAEL	no observed adverse effect level
NOEC	no observed effect concentration
NOEL	no observed effect level
OECD	Organisation for Economic Co-operation and Development
OJ	Official Journal
pH	potential hydrogen -*logarithm* (to the base 10) of he hydrogen ion concentration $\{H^+\}$
pKa	-*logarithm* (to the base 10) of the acid dissociation constant
pKb	-*logarithm* (to the base 10) of the base dissociation constant
Pa	Pascal unit(s)
PEC	predicted environmental concentration
PNEC(s)	predicted no effect concentration(s)
$PNEC_{water}$	predicted no effect concentration in water
(Q)SAR	quantitative structure activity relation
STP	sewage treatment plant
TGD	Technical Guidance Document[2]
UV	ultraviolet region of spectrum
UVCB	Unknown or Variable composition, Complex reaction products or Biological material
v/v	volume per volume ratio
w/w	weight per weight ratio

[2] Commission of the European Communities, 1996. Technical Guidance Document in Support of the Commission Directive 93/67/EEC on risk assessment for new substances and the Commission Regulation (EC) No 1488/94 on risk assessment for existing substances. Commission of the European Communities, Brussels, Belgium. ISBN 92-827-801[1234]