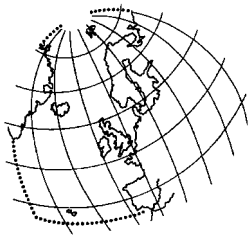
Hazardous Substances Series

4-*tert*-butyltoluene*



OSPAR Commission

2003 (2005 Update)

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* OSPAR 2005 agreed to deselect 4-tert-butyltoluene from the List of Chemicals for Priority Action (OSPAR 05/21/1, §7.5a)

The Convention for the Protection of the Marine Environment of the North-East Atlantic (the "OSPAR Convention") was opened for signature at the Ministerial Meeting of the former Oslo and Paris Commissions in Paris on 22 September 1992. The Convention entered into force on 25 March 1998. It has been ratified by Belgium, Denmark, Finland, France, Germany, Iceland, Ireland, Luxembourg, Netherlands, Norway, Portugal, Sweden, Switzerland and the United Kingdom and approved by the European Community and Spain.

La Convention pour la protection du milieu marin de l'Atlantique du nord-est, dite Convention OSPAR, a été ouverte à la signature à la réunion ministérielle des anciennes Commissions d'Oslo et de Paris, à Paris le 22 septembre 1992. La Convention est entrée en vigueur le 25 mars 1998. La Convention a été ratifiée par l'Allemagne, la Belgique, le Danemark, la Finlande, la France, l'Irlande, l'Islande, le Luxembourg, la Norvège, les Pays-Bas, le Portugal, le Royaume-Uni de Grande Bretagne et d'Irlande du Nord, la Suède et la Suisse et approuvée par la Communauté européenne et l'Espagne.

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EXECUTIVE SUMMARY

4-*tert*-butyltoluene is a neutral organic chemical. It is used primarily as a raw material in the commercial production of p-*tert*-butylbenzoic-acid, which is utilised in the manufacture of unsaturated polyesters and alkyd resins. 4-*tert*-butyltoluene is produced in a closed system and is transported within the plant via pipes to a processing plant where it is entirely transformed in closed production facilities into secondary products through industrial chemical synthesis. According to industry, there are no open uses of 4-*tert*-butyltoluene. On the basis of the product registers of the Nordic countries, Finland, Sweden and Norway confirmed that 4-*tert*-butyltoluene is not registered. The Swiss Product Register lists 4-*tert*-butyltoluene in two products (as a glue or sealing agent and as an auxiliary chemical) with a content of far less than 1% in each of the products.

4-*tert*-butyltoluene is produced in a volume of 1 000-5 000 tonnes/year at the only European production site in Ludwigshafen, Germany.

4-*tert*-butyltoluene is "not readily biodegradable" and is therefore considered to be potentially persistent. Based on its octanol – water-partitioning coefficient (log P_{OW} value), a high potential for bioaccumulation can be assumed. It further shows a low acute aquatic toxicity. The data presented in the background document show that 4-*tert*-butyltoluene has a hazard potential, resulting from its properties with respect to its liability to bioaccumulate and persistence. Since this substance is practically not expected to occur in the environment in significant amounts, the risk for the marine environment is considered low.

At present, there is no need for OSPAR to propose measures for the reduction of emissions of 4-*tert*-butyltoluene. The action recommended is to avoid any new open/and or widely dispersive uses of 4-*tert*-butyltoluene; to invite industry to report any new information on existing open and/or widely dispersive uses of 4-*tert*-butyltoluene and any changes in the use of 4-*tert*-butyltoluene, especially if the changes in use result in an open and/or wide dispersive use; OSPAR to communicate this background document to the European Commission and to other appropriate international organisations which deal with hazardous substances to take account of this background document in a consistent manner.

A monitoring strategy for 4-*tert*-butyltoluene is annexed to this background document.

RECAPITULATIF

Le 4-*tert*-butyltoluène est un produit chimique organique neutre. Il sert essentiellement de matière première pour la fabrication commerciale d'acide p-*tert*-butylbenzoïque, lequel est utilisé pour fabriquer des polyesters non saturés et des résines alkydes. Le 4-*tert*-butyltoluène est fabriqué en circuit fermé et est acheminé par des tuyauteries à l'intérieur de l'usine jusqu'à une installation de traitement où il est entièrement transformé, dans des équipements de fabrication en circuit fermé, en produits secondaires par synthèse chimique industrielle. Selon les dires de l'industrie, le 4-*tert*-butyltoluène n'est pas utilisé en circuit ouvert. Ayant consulté les nomenclatures de produits des pays nordiques, la Finlande, la Suède et la Norvège ont confirmé que le 4-*tert*-butyltoluène n'était pas enregistré. Dans la Nomenclature suisse des produits, le 4-*tert*-butyltoluène est classé dans deux catégories de produits (comme colle ou agent d'étanchéité, et comme produit chimique auxiliaire), sa teneur étant inférieure à 1 % dans chacun des produits.

La production du 4-*tert*-butyltoluène se situe entre 1 000 et 5 000 tonnes par an, la seule unité européenne de fabrication se trouvant à Ludwigshafen, en Allemagne.

Le 4-*tert*-butyltoluène n'est « pas directement biodégradable », et il est donc considéré comme potentiellement persistant. Compte tenu de son coefficient de partage octanol-eau (valeur log P_{OW}), il est présumé que son potentiel de bioaccumulation est élevé. Il présente de plus une faible toxicité aiguë en milieu aquatique. Les données présentées dans le document de fond indiquent que le 4-*tert*-butyltoluène est potentiellement dangereux, en raison de sa faculté de bioaccumulation et de sa persistance. Cette substance ne devant pratiquement pas être présente dans l'environnement en quantités significatives, le risque pour le milieu marin est considéré comme faible.

Pour l'heure, il n'est pas nécessaire qu'OSPAR propose des mesures qui viseraient à réduire les émissions de 4-*tert*-butyltoluène. L'action recommandée consiste à : éviter toute nouvelle application en circuit ouvert et/ou toute utilisation très dispersive du 4-*tert*-butyltoluène de manière à prévenir les risques qui découleraient dans l'avenir des modifications de son utilisation ; inviter l'industrie à communiquer tout nouvel élément d'information sur les applications actuelles en circuit ouvert et/ou très dispersives du 4-*tert*-butyltoluène ainsi que tout changement intervenant dans son utilisation, surtout si ces modifications aboutissent à une utilisation en circuit ouvert et/ou très dispersive ; ce qu'OSPAR communique le présent document de fond à la Commission européenne et aux autres organisations internationales compétentes chargées des substances dangereuses, afin qu'elles tiennent compte du présent document de fond dans des conditions cohérentes.

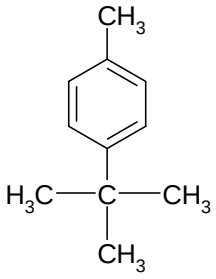
Une stratégie de surveillance sur le 4-*tert*-butyltoluène est annexée à ce document de fond.

1. INTRODUCTION

4-*tert*-butyltoluene is a neutral (pH) organic chemical. It is a clear flammable liquid with a distinct, aromatic, gasoline-like odour. Human volunteers exposed to several concentrations immediately recognised the odour at concentrations as low as 5 ppm (30,5 mg/m³) (quoted in HEALTH COUNCIL OF THE NETHERLANDS 2002). Other sources give the threshold for odour reception at 10 ppm (60mg/m³; Hüls AG substance information).

The chemical identity of 4-*tert*-butyltoluene is presented in Table 1; further physico-chemical data are given in Annex 1.

Table 1: Chemical identity of 4-*tert*-butyltoluene

CAS-No. 98-51-1 EINECS-No. 202-675-9		4-*tert*-butyltoluene Synonyms: 1-(1,1-dimethylethyl)-4-methyl-benzene; p-*tert*-butyltoluene; 1-methyl-4-*tert*-butylbenzene

2. IDENTIFICATION OF SOURCES OF 4-*TERT*-BUTYLTOLUENE AND ITS PATHWAYS TO THE MARINE ENVIRONMENT

2.1 Production of 4-*tert*-butyltoluene and main uses

The only producer in Europe has provided information on the production volume, uses and emissions.

4-*tert*-butyltoluene is produced in a volume of 1 000-5 000 tonnes/year at the one and only European production site in Ludwigshafen, Germany.

4-*tert*-butyltoluene is produced in a closed system and is transported within the plant via pipes to a processing plant where it is entirely transformed in closed production facilities into secondary products through industrial chemical synthesis. According to industry, there are no open uses of 4-*tert*-butyltoluene. The main use category is therefore given as "non-dispersive use".

4-*tert*-butyltoluene is used primarily as a raw material in the commercial production of p-*tert*-butylbenzoic-acid, which is utilised in the manufacture of unsaturated polyesters and alkyd resins.

Finland, Sweden and Norway have confirmed that 4-*tert*-butyltoluene does not appear in their Products Registers. The Swiss Product Register lists 4-*tert*-butyltoluene in 2 products (as a glue or sealing agent and as an auxiliary chemical) with a content of far less than 1% in each of the products (information from the Swiss Federal Health Agency). This is considered to be insignificant for the marine environment.

Reports that 4-*tert*-butyltoluene has other uses, such as an oil additive, solvent, and perfume fixative, which would suggest the potential for consumer exposure, could not be confirmed any further (FIELDEN, 1982; quoted by TOXLINE special; see also HEALTH COUNCIL OF THE NETHERLANDS 2002).

The distribution of 4-*tert*-butyltoluene in Mackay Level I model (Table 2; IUCLID-Dataset 19.2.2000) gives an impression of the affinity of the substance to different compartments and can be a basis for the hazard assessment. The model calculation suggests that the substance enters the environment in a large amount. This is, however, not the case, due to the actual production and use conditions as outlined above.

Table 2: Calculated distribution of 4-*tert*-butyltoluene to different compartments in a Mackay Level 1 model (IUCLID Data Set 19.02.2000)

Compartment	Percentage of substance distributed
Air	60,9 %
Soil	15,7 %
Water	8,8 %
Sediment	14,7 %
Biota	0,01 %

High vapour pressure and low water solubility (see Annex 1) promote a partition into air; this is even more pronounced when calculating the distribution according to the EURAM model (HANSEN ET AL. 1999). This indicates that air transport and oxidative degradation would become important, if 4-*tert*-butyltoluene entered the environment through leakage, spill or open use.

Further, a high log P_{OW} would support adsorption to soil and sediment.

3. MONITORING DATA, QUANTIFICATION OF SOURCES AND ASSESSMENT OF THE EXTENT OF PROBLEMS

3.1 Quantification of sources

3.1.1 Emissions to the atmosphere

Industry reported that information on emissions have been provided to the competent authority in Germany and collected in a register since 1996. According to the declaration of emissions, at Ludwigshafen (Germany) 480 kg of 4-*tert*-butyltoluene were emitted to the air in 2000.

As from 2001 the production of 4-*tert*-butyltoluene was modernised. Since then 4-*tert*-butyltoluene is handled in closed systems throughout the entire production, transport, and further processing procedure. Gaseous 4-*tert*-butyltoluene is vented and directed to a central combustor. Therefore, according to industry, there are only diffuse emissions in quantities, which are so small that they cannot be quantified.

Based on this information it can be concluded that the airborne inputs of 4-*tert*-butyltoluene to the marine environment are negligible.

3.1.2 Riverine inputs

Since there is only one production site for 4-*tert*-butyltoluene in Europe (Ludwigshafen, Germany), and since there are no open uses of 4-*tert*-butyltoluene, the only discharges conceivable to a river (the Rhine in this case) are those via the factories' sewage treatment plant (STP).

The concentration of 4-*tert*-butyltoluene is measured in the inflow and outflow of the STP on a daily schedule with Head Space Gas Chromatography (24 h mixed sample). According to industry, discharges of 4-*tert*-butyltoluene from this plant to the river Rhine, if any, meet the German legal requirements. They

are below the limit values imposed, i.e., 500 µg/l in the inflow of the STP and 20 µg/l in the outflow of the STP, measured by GC. This was verified by all 356 samples taken in 2001 (all below 500 and 20 µg/l, respectively).

Considering a limit value of 20 µg/l and an average output of 5 m³/sec from the STP and a minimum flow of 734 m³/sec of the River Rhine at Ludwigshafen (water gauge Worms), a 150-fold dilution is achieved resulting in calculated concentrations of less than 0,14 µg/l at this point of the river.

Based on this information it can be concluded that the riverine inputs of 4-*tert*-butyltoluene to the North Sea and the North East Atlantic are negligible.

3.1.3 Monitoring data

Besides the measurements at the sewage treatment plant of the production site mentioned above, there are no other monitoring data available for 4-*tert*-butyltoluene.

3.2 Assessment of the extent of the problem

3.2.1 Physico-chemical properties

Representative physico-chemical data of 4-*tert*-butyltoluene are presented in Annex 1.

3.2.2 Biotic and abiotic degradation

Aerobic biodegradation

A test (1995) according to Council Directive 92/69/EEC (C.4-C; equivalent to OECD 301 B, Modified Sturm Test) results in 3% CO_2-evolution in 28 days. This test was performed under GLP and is considered valid according to the test guideline (e.g. with respect to performance and activity of micro-organisms). A substance can only be considered to be readily biodegradable if the endpoint value (in this case CO_2-evolution as a measure of the degree of biodegradation) is higher than a certain pass level (in this case 60% of the theoretically expected CO_2-evolution). Since CO_2-evolution for 4-*tert*-butyltoluene was far lower than the pass level, 4-*tert*-butyltoluene is characterised as "not readily biodegradable" (IUCLID Data Set 19.2.2000).

Another, earlier test (1989; non-GLP) according to OECD-Guideline 301 D (Closed Bottle Test) results in 7% O_2-consumption. Since the pass level is not reached either, 4-*tert*-butyltoluene is also characterised as "not readily biodegradable" in this test (IUCLID Data Set 19.2.2000).

In a test on inhibition of oxygen consumption with the bacterium *Pseudomonas putida* (1995; GLP; Hüls-Method) it was shown that 4-*tert*-butyltoluene does not inhibit the metabolism of bacteria in a concentration range of 1 mg/l to 1 000 mg/l (the test item was kept in suspension by stirring). The low biodegradability stated above can therefore not be attributed to a toxicity to bacteria.

This type of screening tests does not allow the estimation of half-lives. However, according to the revised Technical Guidance Document (TGD) [1], when results from biodegradation tests simulating the conditions

[1] The Technical Guidance Document (TGD) was revised and has been published in April 2003. It contains a new chapter on marine risk assessment and criteria for the assessment of persistence, bioaccumulation potential and toxicity (PBT) of substances, which may pose a risk for the marine environment. Risk assessment in this background document follows the PBT assessment scheme in the revised TGD, a draft of which has already been available in the 2nd half of 2002. This risk assessment methodology has been formally agreed by the EC in April 2003 and has been adopted by the OSPAR Commission in June 2003 as the common EU/OSPAR risk assessment methodology for the marine environment.

in surface waters are not available, the use of results from various screening tests may be considered, and mineralisation half-lives (days) are recommended according to the outcome of degradation screening tests. A substance, which is "not readily biodegradable", is to be considered to have an indefinite half-life. According to the marine PBT assessment (revised TGD, 2003; Chapter 3, Sections 4.2.3.4, 4.4.2 and 4.4.3.5) it is suggested that, in the absence of other biodegradation tests, in particular simulation tests in freshwater and/or saltwater, a characterisation as "persistent" or "very persistent" may be derived from the screening test result.

Atmospheric and abiotic degradation

The specific degradation rate constant of 4-*tert*-butyltoluene with hydroxyl radicals in the atmosphere was calculated to $6,7*10^{-12}$ cm³/molecule*sec from the structure of the molecule. From this, the pseudo-first-order rate constant for degradation in air can be calculated according to the TGD (Chapter 2.3.6, 24 h day, $5* 10^5$ OH/cm³) to 0,29. The resulting half-life of 2,4 days corresponds to 57,5 hours. The half-life estimation in the IUCLID dataset is 2,2 days which corresponds well with the calculation above. A half-life of more than 1 day is considered relevant for the marine environment by OSPAR, while the trigger for POPs is considered to be at a half-life of 2 days.

4-*tert*-butyltoluene is a rather volatile substance (vapour pressure 80 Pa at 20 °C). Although photo-oxidative degradation is fairly rapid, the persistence of 4-*tert*-butyltoluene in air has to be considered relevant for the OSPAR Convention area, considering the short distance from the European continent to the North East Atlantic, provided that relevant emissions to air would occur.

There is no information on hydrolysis of 4-*tert*-butyltoluene available.

3.2.3 Bioaccumulation

Information on bioaccumulation (in terms of bioconcentration, BCF) for 4-*tert*-butyltoluene can be derived from the log P_{OW}. With the method of MEYLAN ET AL. (1999) BCFs can be calculated as follows:

$$\log BCF = 0,77 * \log P_{OW} - 0,70;$$

no correction factors to be applied. In Table 3, BCF calculations are summarised.

The method of MEYLAN ET AL. (1999) is improved against the method of VEITH ET AL. (1979), which is:

$$\log BCF_{fish} = 0,85 * \log P_{OW} - 0,70.$$

However, VEITH ET AL. (1979) is mentioned in the TGD (rev. 2003; Chapter 3, Section 3.8.3.2 and Chapter 4 on the use of QSARs). The method of VEITH ET AL. (1979) generally results in higher BCF values, e.g. using a log P_{OW} of 4,45 would result in a BCF of 1 209.

Table 3: BCF values for 4-*tert*-butyltoluene, calculated from log P_{OW} values

log P_{OW}	Source of log P_{OW}	Calculated BCF	Calculation method for BCF	Remarks
4,35	IUCLID dataset Huels AG, 1981	446	MEYLAN ET AL. 1999	Standard deviation of measurement of log Pow : 4,23-4,45
4,45	KOWWIN v1.66	533	MEYLAN ET AL. 1999	
		1 905	OSPAR Fact sheet	
(5,17)	MITI (1992) OSPAR Fact sheet	(1 909)	MEYLAN ET AL. 1999	log P_{OW} estimation method unknown
		2 320 (should be disregarded)	?	Initial selection criterion; not stated in actual fact sheet

The first OSPAR Fact Sheet stated a calculated BCF of 2 320 from ECB database (European Chemicals Bureau, Ispra, Italy). The initial selection was based on this QSAR. However, this value is not stated in the revised fact sheet anymore and should be disregarded.

The derivation of the log P_{OW} of 5,17 from the MITI handbook, which is stated in the OSPAR fact sheet, could not be sufficiently clarified. Therefore, this value and subsequent BCF calculations derived from it should be disregarded.

The log P_{OW} value of > 4 itself indicates a "high potential for bioaccumulation". A substance is considered to potentially fulfil the B-criterion in the marine PBT assessment when the log P_{OW} exceeds 4,5.

Experimental BCF data are not available.

Taking all information into account, 4-*tert*-butyltoluene has a high potential for bioaccumulation (which triggered the initial selection), but acceptable calculated BCF values are just below the trigger of BCF > 2 000. The acceptable log P_{OW} values are also just below the trigger of 4,5. With respect to the B-criterion, 4-*tert*-butyltoluene can be considered as a borderline case. Following the marine PBT assessment as is, would lead to the conclusion that the B-criterion is just not met.

Considering the uncertainty of QSAR estimations, it might be advisable to perform an experiment on bioconcentration in fish, or possibly – because of the relatively high hydrophobicity – in sediment dwelling organisms. However, the requirement for such a test should be triggered by the risk of occurrence in the marine environment, which appears to be insignificant for 4-*tert*-butyltoluene.

3.2.4 Acute and chronic ecotoxicity effects

Some data on ecotoxicity of 4-*tert*-butyltoluene are given in the following Tables 4 and 5.

Table 4: Data on the ecotoxicity of 4-*tert*-butyltoluene

4-*tert*-butyltoluene (CAS No. 98-51-1)					
Test organism	**Trophic level / Habitat**	**Endpoint / Effect**	**Test conditions**	**Endpoint concentration**	**Source Year**
Pseudomonas putida	Micro-organism FW	EC_{50} O_2-consumption	5 h own meth; GLP	> 1 000 mg/l	[1] 1995
Scenedesmus subspicatus	pProd FW	NOEC GRO, BioM	3 d; STA; EC 92/69/; GLP	> 5,6 mg/l	[1] [a] 1992
Daphnia magna	pCons FW	LC_{50} IMM	2 d; STA; EC 92/69/; GLP	3,2 mg/l	[1] 1992
Cyprinus carpio	sCons FW	LC_{50} MOR	4 d; REN; EC 92/69/; GLP	2,0 mg/l	[1] 1992
Carassius auratus	sCons FW	LC_{50} MOR	1 d; STA; APHA 1971	3,0 mg/l	[2] 1979
Leuciscus idus	sCons FW	LC_{50} MOR	2 d; STA; DIN 38412, 15	9,9 mg/l	[1] 1987
Xenopus laevis	sCons FW	LC_{50} MOR	2 d; STA;	5,0 mg/l	[3] 1987

[1] In IUCLID Data Set (Rev. 19.2.2000); EURAM effects database at the ECB (Ispra, Italy).

[2] BRIDIÉ ET AL. (1979); Water Res. 13: 623-626; quoted in AQUIRE.

[3] DE ZWART & SLOOF (1987); Bull. Environ. Contam. Toxicol 38:345-351; quoted in AQUIRE.

pProd: primary producers; pCons: primary consumer; sCons: secondary consumer; FW: freshwater species; SW: saltwater species; GRO: Growth; MOR: Mortality; IMM: Immobilisation; STA: static test; REN: semi-static (renewal) test; ACT: active substance; FORM: Formulation instead of active substance was used in the test; n.g.: not given.

a) Test duration or other important parameter missing or not standard (acc. to ECB).

The tests listed in the IUCLID dataset have mostly been conducted under GLP and in accordance with EU- or OECD-guidelines. The test with the bacterium *Pseudomonas putida* has been mentioned in the context of biodegradation studies and shows that there is no inhibition of bacterial metabolism. In the test with the algae *Scenedesmus subspicatus* under GLP, test concentration was analysed at 0 and 72 hours and showed a decrease of less than 20% of the nominal concentration. Reporting the NOEC endpoint with respect to the nominal concentration is therefore valid. In the test with *Daphnia magna* (under GLP) deviation of the measured concentrations was larger than 20% of the nominal concentrations. Therefore, evaluation was done with respect to the geometric mean or the test with *Leuciscus idus* there is no confirmation of measured concentration data available and this was a non-GLP test. The reported EC_{50} (48 h) of 9,9 mg/l must have therefore been based on a nominal concentration.

The test on the goldfish (*Carassius auratus*) described by BRIDIÉ ET AL. (1979) was conducted in accordance with guidelines laid down by the American Public Health Association (APHA, 1971). Test conditions (e.g. 10 healthy fish at 20 °C, not aerated) are reported completely, including a control of the test solutions (DOC or GC analysis). The test result appears to be valid and is in the range of other results from fish.

For the tests on *Carassius auratus* (BRIDIÉ ET AL. 1979) and the test on *Xenopus laevis* (DE ZWART & SLOOF 1987) described in the following paragraph, the authors have accounted for the medium volatility (according to Henry's coefficient of $5{,}20*10^{-4}$ to $1{,}62*10^{-3}$ [-]) by not aerating and covering the glass aquaria. Therefore loss by evaporation is limited.

BRIDIÉ ET AL. (1979) reported that the concentration of the test substance in the vessels was measured before and after each test with a total organic analyser or by extraction and subsequent GC analysis.

However differences between these two measurements are not reported; therefore the endpoint concentration of 3,0 mg/l can be considered as nominal concentration.

The test on the clawed toad (*Xenopus laevis*) is described by DE ZWART & SLOOF (1987). Several chemicals were investigated in this study and the acute toxicity (LC_{50}) was assessed for each of the chemicals individually. Test conditions are described in detail (e.g. 10 3-4 weeks old larvae at 20 °C, 5 concentration levels having a factorial difference of 1,5 covered glass aquaria), although no reference is made to a test guideline.

DE ZWART & SLOOF (1987) give details on the preparation of the test solutions but not on a chemical analysis after the test. Therefore the endpoint concentration of 5,0 mg/l can be considered as nominal concentration.

Both values are in the range of the water solubility of 4-*tert*-butyltoluene (10-600 mg/l; cf. Annex 1), which gives reason to the assumption that the effective concentrations reach the nominal concentrations in the tests.

Several lower chronic ecotoxicity concentrations are reported in the OSPAR Fact Sheet by the ECB (European Chemicals Bureau) (Table 5), which are QSAR values. These QSARs flag the toxicity of 4-*tert*-butyltoluene for aquatic organisms but should only be considered if no experimentally determined data are available. The chronic values are not below the 0,01 mg/l threshold.

Further QSAR ecotoxicity values are reported in the OSPAR fact sheet. Fathead Minnow model: acute LC_{50} 3,2 mg/l; *Daphnia* model: acute EC_{50} 0,42 mg/l; Lethal body burden NOEC for fish based in EPIWIN 3.02 BCF: 0,0634 mg/l. As stated before, QSARs are not taken into consideration if measured data are available (see Table 3).

From the experimental ecotoxicity data (Table 4) follows that 4-*tert*-butyltoluene is acutely toxic to aquatic organisms, but does *not* meet the T-criterion (< 0,1 mg/l for acute ecotoxicity according to marine PBT criteria). The lowest reported acute toxicity is 2,0 mg/l (nominal; in the range of water solubility) and thus far higher than the trigger of 0,1 mg/l mentioned.

Table 5: QSAR-data on the ecotoxicity of 4-*tert*-butyltoluene (OSPAR fact sheet)

4-*tert*-butyltoluene (CAS No. 98-51-1)					
Test organism	**Trophic level / Habitat**	**Endpoint / Effect**	**Test conditions**	**Endpoint concentration**	**Source Year**
Algae	pProd FW	Acute toxicity	n.g. QSAR	0,2978 mg/l	[4]
Daphnia	pCons FW	Acute toxicity	n.g. QSAR	0,5462 mg/l	[4]
Daphnia	pCons FW	Chronic toxicity	n.g. QSAR	0,06688 mg/l	[4]
Fish	sCons FW	Chronic toxicity	n.g. QSAR	0,08604 mg/l	[4]

[4] Data from OSPAR Fact Sheet (NSDB/ECB).

pProd: primary producers; pCons: primary consumer; sCons: secondary consumer; FW: freshwater species; n.g.: not given.

3.2.5 Carcinogenicity, mutagenicity or harmful reproductive effects

A health-based assessment of 4-*tert*-butyltoluene was conducted by a committee of the HEALTH COUNCIL OF THE NETHERLANDS (2002).

4-*tert*-butyltoluene did not induce mutations in bacteria (*S. typhimurium*, *E. coli*), gene conversion in yeast (*S. cerevisiae*), or chromosome damage in mammalian cells (rat liver RL_1 cells). No data were found on in vivo genotoxicity testing (*ibid*.).

The Committee did not find adequate studies on the potential reproduction toxicity of 4-*tert*-butyltoluene, but the available data indicate that exposure to 4-*tert*-butyltoluene might induce developmental toxicity. In rats, germinal epithelial damage was seen after 5 daily oral doses of 50 and 100 mg/kg body weight (bw), but not at 25 mg/kg bw. Similar damage was observed in mice and to a lesser degree in guinea pigs and dogs at doses of 100 mg/kg bw (no other doses were tested; *ibid*.).

The Committee did not find data on the potential carcinogenicity of 4-*tert*-butyltoluene.

3.2.6 Toxicological effects

Human toxicological effects of 4-*tert*-butyltoluene are also discussed in (HEALTH COUNCIL OF THE NETHERLANDS 2002).

4-*tert*-butyltoluene is readily absorbed from the respiratory and gastrointestinal tract, rapidly distributed throughout the body and after being metabolised, excreted in urine and faeces within a few days (*ibid*.). Following exposure, several mild and transient irritating effects were observed in humans.

Based on experimental animal data, it is concluded that liquid 4-*tert*-butyltoluene is at most slightly irritating to eyes and skin. The compound did not show sensitising properties when tested in the maximisation test in guinea pigs (*ibid*.).

From acute lethality (LD_{50}) data, 4-*tert*-butyltoluene is considered toxic by inhalation and harmful if swallowed while no such qualification is warranted as to dermal exposure (*ibid*.).

Acute repeated inhalation experiments in rats and rabbits showed that irritation of eyes and respiratory tract and effects on the nervous system are predominant and that chronic exposure may induce slight effects on the liver (*ibid*.).

3.3 Risk to the environment

4-*tert*-butyltoluene was selected as priority substance according to the DYNAMEC criteria partly based on QSAR data. Revision of data and application of the risk assessment based on the criteria as outlined in the revised Technical Guidance Document (see section 2.2.2) have led to the following assessment of the substance.

4-*tert*-butyltoluene showed to be "not readily biodegradable". Since no other biodegradation tests were available, this screening test result may be used to evaluate the P-criterion according to the marine PBT assessment in the revised TGD. Further, due the high volatility of the substance and a certain persistence in air (half life around 2 days), there is a potential for transport from the continent to the sea. Therefore, 4-*tert*-butyltoluene is considered to be potentially persistent (P-criterion or vP-criterion fulfilled).

From the log P_{OW} (4,35-4,45) 4-*tert*-butyltoluene possesses a high potential for bioaccumulation. The log P_{OW} of 4,45 is very close to the trigger of 4,5 in the marine PBT assessment. QSARs of the bioaccumulation factor range from 446 to 1 905. Higher BCF calculations do not seem reliable. Therefore, the B-criterion is just not met. However, the calculated BCFs of up to 1 905 are also very close to the threshold of BCF > 2 000 in the marine PBT assessment.

The experimentally determined acute ecotoxicity of 4-*tert*-butyltoluene for aquatic organisms from different trophic levels shows, that 4-*tert*-butyltoluene is toxic to this group of organisms. QSAR data indicate a high potential of toxicity for aquatic organisms, but, nevertheless, the T-criterion (0,1 mg/l for an acute ecotoxicity; cf. PBT assessment) is not met.

With respect to the criteria for very persistent and very bioaccumulative (vPvB) substances, as set out in the marine PBT assessment, 4-*tert*-butyltoluene can be considered as a borderline case. A half-life has not been determined, but persistence is evaluated on the basis of a "not readily biodegradable" screening test result. From this, an assignment "very persistent" can be made. However, bioaccumulation, in terms of a (calculated) BCF, is slightly below the trigger of 2 000 and does by far not reach the value of 5 000 for "very bioaccumulative" substances. On the other hand, the log P_{OW} nearly reaches the trigger of 4,5 which indicates that the substance has a high potential for bioaccumulation.

The evaluation of CMR-toxicity data by the HEALTH COUNCIL OF THE NETHERLANDS (2002) indicates that there is no significant hazard potential of long-term toxicity for humans.

Further, the presently available information on uses, as provided by industry and several Product Registers, indicates to a sufficient degree that 4-*tert*-butyltoluene is only used as intermediate in closed processing systems. Emissions from the production process into the air or from the sewage treatment plant of the production site into the river Rhine are below the limit value. Under normal operational conditions, there is no contact to the environment of 4-*tert*-butyltoluene in production and waste-disposal. Except in the case of an accident, it is very unlikely that 4-*tert*-butyltoluene will enter the environment and lead to a marine exposure.

The data presented here show that there is a hazard potential by 4-*tert*-butyltoluene, resulting in particular from its persistence and bioaccumulative properties, but since this substance is practically not expected to occur in the environment in significant amounts, the risk for the marine environment is lower than anticipated.

4-*tert*-butyltoluene cannot be considered to be a PBT- or vPvB-substance to a full extent, and a performance of a quantitative marine risk assessment (PEC/PNEC-risk quotients) does not seem appropriate, since this substance is practically not expected to occur in the environment in significant amounts due to its use in closed systems only.

4. DESIRED REDUCTION

According to its intrinsic properties, especially its toxicity to aquatic organisms, 4-*tert*-butyltoluene has been selected by OSPAR on the List of Substances of Possible Concern, and prioritised in 2001. Its deliberate release into the marine environment should be avoided.

However, since it is used entirely as an intermediate in closed production, as far as has become known, there is presently no indication of a marine exposure.

Therefore, no reduction objective is presently provided. Open uses should be also avoided in future, but if 4-*tert*-butyltoluene should be used in an open application or in a matrix, appropriate measures should be taken to avoid entry into the marine environment.

5. REVIEW OF AGREED MEASURES AND POSSIBLE SUBSTITUTES

5.1 Review of agreed national and international measures for the regulation of 4-*tert*-butyltoluene

OSPAR Strategy with regard to Hazardous Substances

4-*tert*-butyltoluene was selected in the DYNAMEC process early in 2000. At the meeting of the OSPAR Commission held in Copenhagen in June 2000, 4-*tert*-butyltoluene was agreed as a priority substance and Germany volunteered to take the lead in the preparation of the background document. Under the assumption that 4-*tert*-butyltoluene is used exclusively as an intermediate in closed production systems, OSPAR's Working Group on Priority Substances agreed in 2001 that the background document should be prepared in an abbreviated manner ("tailored approach"). The working group provided evidence to underpin that assumption.

Council Regulation (EEC) No. 793/93 of 23 March 1993 on the evaluation and control of the risks of existing substances

Under the Regulation (EEC) 793/93, 4-*tert*-butyltoluene has been included in the EINECS list of existing substances produced or imported within the Community in quantities exceeding 1 000 tonnes per year and appropriate data reporting has been established.

Administrative rules concerning substances hazardous to water

4-*tert*-butyltoluene is classified as "hazardous to water" (Water Hazard Class 2/ Wassergefährdungsklasse 2) under the German Administrative Regulation relating to Substances Hazardous to Water (Verwaltungsvorschrift wassergefährdende Stoffe; Bundesanzeiger Nr. 51, 98a, 1 (1999); cf. Legal File http://irptc.unep.ch/irptc/legint.html). The purpose of the classification is to identify the technical requirements of industrial plants, which handle substances hazardous to water.

Other administrative rules / Occupational exposure limits

The HEALTH COUNCIL OF THE NETHERLANDS (2002) gives an overview of occupational exposure limits for 4-*tert*-butyltoluene in various countries. The limits reach from 1 ppm (6,1 mg/m³) in 8 h (Netherlands, Denmark) to 20 ppm (120 mg/m³) in 15 min (USA – NIOSH). However, the Committee considers the

toxicological database on 4-*tert*-butyltoluene too poor to justify recommendation of a health-based occupational exposure limit, although it appears that the present MAC[2]-value may be too high.

In the German List of MAK and BAT Values (maximum concentrations and biological tolerance occupational exposure limits), 4-*tert*-butyltoluene is placed in Section IIb: Substances for which no MAK value (for air) can be established at present because studies on the effects in man or in experimental animals have yielded insufficient information (see Legal File http://irptc.unep.ch/irptc/legint.html).

Nevertheless, the German Technical Rules for Hazardous Substances (TRGS) that deal with limit values for air at the workplace (Technische Regeln für Gefahrstoffe - Grenzwerte in der Luft am Arbeitsplatz – TRGS 900; available in German only) established limit values of 10 ml/m³ or 60 mg/m³. Due to insufficient data, these limit values are preliminary.

5.2 Choice of substitutes

For the intended uses of 4-*tert*-butyltoluene (see Section 1.1), substitutes are not known.

6. CHOICE FOR ACTION/MEASURES

From the available information, it has become clear that 4-*tert*-butyltoluene is produced and used entirely in closed systems, and that it is transported only within a single processing plant in pipes. The data presented in this background document show that there is a hazard potential by 4-*tert*-butyltoluene, resulting from its P and B properties, but since this substance is not expected to occur in the environment in significant amounts due to its use in closed systems, the risk for the marine environment, as assessed according to the criteria stated in the revised marine risk assessment scheme in the revised TGD, is lower than anticipated.

Conclusion on the avoidance of future risks

At present, there is no need for OSPAR to propose measures for the reduction of emissions of 4-*tert*-butyltoluene.

In order to avoid any future risks that might result from changes in use of 4-*tert*-butyltoluene,

- Contracting Parties should avoid any open/and or widely dispersive uses of 4-*tert*-butyltoluene;
- OSPAR should invite Contracting Parties to report any changes in the use of 4-*tert*-butyltoluene, especially if the changes in use result in an open and/or widely dispersive use;
- OSPAR should invite industry to report significant changes in the production volume and in the use of 4-*tert*-butyltoluene to OSPAR, so that the evaluation of the risk to the marine environment can be reviewed, if necessary.

In order to avoid future risks resulting from the use of 4-*tert*-butyltoluene as intermediate,

- OSPAR should invite Contracting Parties to check that the operation of plants using 4-*tert*-butyltoluene is controlled according to the principles of BAT (Best Available Techniques) and that any releases are eliminated or minimised to the greatest extent possible.

[2] MAC: maximum allowable concentration

The need for consistency in actions by other bodies

To ensure that the information in this background document and the conclusions reached by OSPAR are taken into account in the approach of the European Community,

- OSPAR should communicate this background document to the European Commission for information.

To ensure that the information in this background document can be considered in the context of other international agreements which deal with hazardous substances, and with which Contracting Parties are associated,

- OSPAR should send copies of this background document to the appropriate bodies dealing with those agreements and invite Contracting Parties who are parties both to OSPAR and those other agreements to promote action to take account of this background document by those other international bodies in a consistent manner.

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ANNEX 1: PHYSICO-CHEMICAL PROPERTIES OF 4-*TERT*-BUTYLTOLUENE

Property	Value	Source
Chemical name	4-*tert*-butyltoluene	IUCLID Data Set (19/2/2000)
CAS-No.	98-51-1	IUCLID Data Set (19/2/2000)
EEC No. (EINECS)	202-675-9	IUCLID Data Set (19/2/2000)
Molecular formula	C_{11} H_{16}	IUCLID Data Set (19/2/2000)
Molecular Mass M [g/mol]	148,25	
Physical state of matter at 20 °C	liquid	IUCLID Data Set (19/2/2000)
Colour / odour	clear / aromatic	HEALTH COUNCIL NL 2002
Solubility in water S [g/l]	ca. 0,6 (20 °C) 0,01 0,003 (25 °C)	IUCLID Data Set (19/2/2000) OSPAR fact sheet (MITI 1992) QSAR-DK (EPIWIN 3.02) [3]
Density [g/cm³]	0,86 at 20 °C	IUCLID Data Set (19/2/2000)
log P_{OW}	4,35 (meas.) 4,45 (calc.) 5,17 (meas. ?)	IUCLID Data Set (19/2/2000) QSAR-DK (EPIWIN 3.02/3.20) MITI (1992) in EPIWIN 3.20 [4]
Adsorption coefficient (o.c.) log K_{oc} [l/kg]	3,96 (calc.) 3,28 (calc.)	IUCLID Data Set (19/2/2000) [5] EPIWIN 3.20
Melting point T_m [°C]	- 62,5 - 10	IUCLID Data Set (19/2/2000) EPIWIN 3.20 (mean)
Boiling point T_b [°C]	193 at 1013 hPa 191	IUCLID Data Set (19/2/2000)
Vapour pressure P [Pa]	80 at 20 °C 76	IUCLID Data Set (19/2/2000) QSAR-DK (EPIWIN 3.02)
Henry's Law constant [-]	$5,20 * 10^{-4}$ $6,41 * 10^{-4}$ $1,62 * 10^{-3}$	EPIWIN 3.20 (Bond Method) [6] EPIWIN 3.20 (Group Method) EPIWIN 3.20 (VP/WSol)
Volatilisation from water: Half-life from river model [h] Half-life from lake model [h]	 1,3 (0,05 d) 116,3 (4,85 d)	 EPIWIN 3.10 (using Henry LC $5,20 * 10^{-4}$)

[3] Estimate from log P_{OW} 5,17; an estimate with log P_{OW} 4,35 results in a water solubility of 0,015 g/l (MITI 1992).

[4] This highest log P_{OW} value of 5,17 has been reported in the EPIWIN 3.20 experimental database (MITI 1992). It was used for the calculation of several other parameters in EPIWIN 3.20.

[5] The calculation of the adsorption coefficient K_{oc} according to the IUCLID Data Set is based on the lowest reported log P_{OW} of 4,35 and the KARICKHOFF formula ($K_{oc} \approx 0,41 * P_{OW}$) while EPIWIN 3.20 calculates the K_{oc} on basis of a 1st order molecular connectivity index derived from the structure of the molecule.

[6] All EPIWIN 3.10 estimates for the Henrys law constant are converted from atm*m³/mole to the dimensionless form. 4-*tert*-butyltoluene is to be considered as a volatile substance (also the vapour pressure of 80 Pa at 20 °C).

Property	Value	Source
Reactivity with OH-radicals atmospheric half-life [d]	1,59 2,2	QSAR-DK (EPIWIN 3.20) [7] IUCLID Data Set (19/2/2000)
Hydrolysis half-life [d]	-	EPIWIN 3.20 [8]
Toxicological classif. (EU)	T, N	ICSC 1068
R-Phrases	R 7, 22, 23, 36, 38 51/53	DK-Draft Advisory list for self-classification
S-Phrases	no information	

[7] The atmospheric half-life is calculated on a basis of a 12-hour day and 1,5 * 10^6 OH-radicals/cm³. The choice of parameters which are more common in Europe would result in slightly higher values (cf. IUCLID data set).

[8] EPIWIN 3.20 could not estimate a hydrolysis rate constant for the structure of 4-*tert*-butyltoluene.

ANNEX 2: MONITORING STRATEGY FOR 4-*TERT*-BUTYLTOLUENE

As part of the Joint Assessment and Monitoring Programme (*reference number 2003-22*), OSPAR 2004 adopted an Agreement on monitoring strategies for OSPAR Chemicals for Priority Chemicals (*reference number 2004-15*) to implement the following monitoring for tracking progress towards the objectives of the OSPAR Hazardous Substances Strategy (*reference number 2003-21*) with regard to 4-*tert*-butyltoluene. The Monitoring Strategy for 4-*tert*-butyltoluene will be updated as and when necessary, and redirected in the light of subsequent experience.

4-*tert*-butyltoluene is produced as an intermediate and used in closed systems only. According to industry, there are no open uses of 4-*tert*-butyltoluene. The Swiss Product register lists it in two products only with a content of far less than 1% in each of the products. Therefore, no monitoring of sources of emissions is necessary.

There is only one production site in Europe, in Ludwigshafen, Germany. As from 2001, the production was modernised and emissions to air from this substance with high vapour pressure have become so small that they cannot be quantified. Discharges to the river Rhine via the factory's sewage treatment plant meet the German limit value. Therefore, emissions to the environment are negligible. As a consequence, no monitoring is necessary for the marine environment, since no release to the environment is expected except in the case of accidents only.

OSPAR will, however, seek to estimate quantities of 4-*tert*-butyltoluene imported to, and exported from, the OSPAR region.

Contracting Parties should report any changes to use pattern of 4-*tert*-butyltoluene outside closed systems. In which case the approach of this monitoring strategy will need to be reconsidered bearing in mind that the T criterion is not met for 4-*tert*-butyltoluene.

4-TERT-BUTYLTOLUENE MONITORING STRATEGY	
Implementation of actions and measures	• Examination of progress in the implementation of regulations on marketing and/or use or emission and/or discharge which have been agreed, or are endorsed, by the Background Document
Production/use/sales figures	• Contracting Parties should report any use of 4-*tert*-butyltoluene outside closed systems. Following any such report the need for revision of this monitoring strategy should be considered • Estimate quantities imported to, and exported from, the OSPAR region