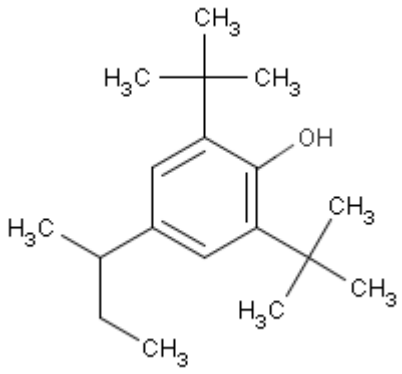
INITIAL TARGETED ASSESSMENT PROFILE

CAS RN	**17540-75-9**
Chemical Name	**Phenol, 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-** (**DTBSBP**)
Structural Formula	

SUMMARY CONCLUSIONS OF THE TARGETED ASSESSMENT

NOTE: The present assessment is targeted to address the following environment endpoints: stability in water and biodegradability, bioaccumulation potential, acute toxicity to aquatic organisms based on read across to close structural analogues and application of (Q)SAR model predictions. It cannot be considered as a full SIDS Initial Assessment. Summary information on exposure is also reported here. Other endpoints for human health and the environment are included in the Canadian screening assessment but have not been agreed upon by OECD member countries, and thus are not included in this profile.
The final screening assessment has been published under the responsibility of the Government of Canada.
[http://www.ec.gc.ca/ese-ees/default.asp?lang=En&n=AE29F426-1]

Rationale for Targeting the Assessment

The Government of Canada "categorized" or prioritized all 23,000 chemical substances on its Domestic Substances List (DSL) from 1999 to September 2006, as required by its *Canadian Environmental Protection Act, 1999* (CEPA 1999). Using information from Canadian industry, academic research and other countries, Government of Canada scientists applied a set of rigorous tools to the 23,000 chemical substances on the DSL. They were categorized to identify those that were: **inherently toxic** to humans or to the environment and that might be **persistent** and/or **bioaccumulative**; and substances to which people might have **greatest potential for exposure**. During this priority-setting exercise, distinct approaches were taken for identifying substances of likely concern for human health and the environment, and subsequent assessment activities may have focused on either human health or ecological endpoints. Through categorization, the Government of Canada has identified approximately 4,000 of the 23,000 chemical substances on the DSL as priorities for further assessment, research and/or measures to control their use or release.

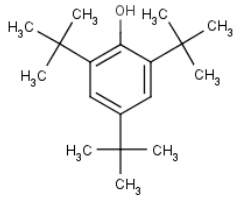
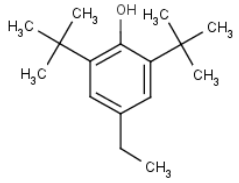
The substance, DTBSBP was identified as a high priority for assessment of ecological risk because it was found to meet the ecological categorization criteria for persistence, bioaccumulation potential and inherent toxicity to aquatic organisms, and was believed to be in commerce in Canada.

Analogue rationale

To fill data gaps for biodegradation, bioaccumulation and ecotoxicity endpoints, a literature search was performed

and the database ChemIDplus® was used to identify appropriate analogue substances of DTBSBP. The substances 2,4,6-tri-*tert*-butylphenol (CAS RN 732-26-3) and 2,6-di-*tert*-butyl-4-ethylphenol (CAS RN 4130-42-1) were found to be appropriate analogues for DTBSBP as they are similar in molecular mass and have similar structure and functional groups to DTBSBP. The molecular mass of DTBSBP is 262.44 g/mol. The structure and molecular mass of these analogue substances are presented in Table 1 below.

Table 1. Analogue substances of DTBSBP used in the assessment

Analogue	Structure	Molecular mass (g/mol)
2,4,6-tri-*tert*-butylphenol, CAS RN 732-26-3		262.4
2,6-di-*tert*-butyl-4-ethylphenol, CAS RN 4130-42-1		234.4

Physical-chemical properties

The substance DTBSBP is a liquid at room temperature. Physical-chemical property data for DTBSBP and analogue substances are presented in Table 2 below.

Table 2. Experimental and modelled physical-chemical properties of DTBSBP and analogue substances[1]

CAS RN.	Log Kow	Water solubility (mg/L)	Melting Point (°C)	Boiling Point (°C)	Vapour Pressure (Pa)
17540-75-9 (DTBSBP)	6.43 (m) **6.1 (m)**	0.25 (m) **2.5 (m)**	102 (m) **18.9 (e)**	330 (m) **275 (e)**	0.0028 (m) **0.35 (m)**
732-26-3	6.39 (m) 6.06 (e)	0.51 (m)	104 (m) 131 (u)	324 (m) 278 (u)	0.027 (m)
4130-42-1	5.52 (m)	2.1 (m)	92 (m) 44 (u)	310 (m) 272 (u)	0.29 (m)

(e= experimental data; m= modelled data; u= unknown: value is from a compilation volume)

1. For a level comparison between all the substances, the first line of data for each substance shows data modelled using EPI Suite (2008) without the input of any available measured physical-chemical properties. The second line of data for each substance gives the measured values, where available, and in the case of DTBSBP, either measured values or values that were modelled using EPI Suite (2008) with some input of

measured or analogue physical-chemical property values. This second line of values in the table for DTBSBP are the values that were used for further modelling of the environmental fate, ecotoxicity and bioaccumulation of this substance. For some of the analogue values, the original source of the data is not actually known as the values were taken from compilation volumes.

Human Health

Not part of the targeted assessment.

Environment

The acid dissociation constant (pK_a) of DTBSBP was modelled using the ACD/pK_aDB Prediction Module (2005, v.9.04). The relatively high value obtained (pK_a = 11.85) for the hydroxyl group of DTBSBP indicates that in water bodies at environmentally relevant pH (6–9), nearly 100% of the substance will be undissociated.

According to the results of Level III fugacity modelling (EQC model 2003, v.2.02), DTBSBP is expected to predominantly reside in sediment (54%) and in air (36%) if released only to air. It will primarily reside in sediment (96%) if released only to water, and in soil (99.9%) if released only to soil.

Based on its high estimated log K_{oc} value of 4.47 (PCKOCWIN, 2000, v.2.00), if released into water, DTBSBP is expected to adsorb strongly to suspended solids and sediment, and if released to soil, it will have high adsorptivity to soil particles (i.e., it is expected to be immobile). An estimated Henry's Law constant of 3.70 $Pa \cdot m^3/mol$ (HENRYWIN, 2000, v.3.20) suggests that volatilization from water surfaces and moist soils is not expected to be high.

Atmospheric degradation of DTBSBP was modelled using AOPWIN (2000, v.1.92). A predicted half-life of 0.52 days via reactions with hydroxyl radicals demonstrates that DTBSBP is likely to be rapidly oxidized. The substance is not expected to react with other photo-oxidative species in the atmosphere, such as O_3.

Since only one experimental study on the biodegradation of DTBSBP was available, read-across analogue data and ultimate biodegradation predicted by models (BIOWIN 2000 v.4.10, TOPKAT 2004 v.6.2, Canadian POPs Model 2008) were also considered. All modelled results agree that that DTBSBP will not biodegrade rapidly and is expected to have a long ultimate degradation half-life in water (months). These ultimate degradation results are consistent with the properties associated with the functional groups in the chemical structure of DTBSBP. The estimated results predicting an ultimate degradation half-life of ≥ 182 days in water are supported by the empirical data that indicate that DTBSBP and its analogue substances, 2,4,6-tri-*tert*-butylphenol and 2,6-di-*tert*-butyl-4-ethylphenol, do not readily biodegrade under aerobic conditions (OECD TG 301C; 0% BOD after 28 days; same result for all three substances). Also, DTBSBP does not contain functional groups expected to undergo hydrolysis in water, and this substance contains structural features associated with chemicals that are persistent (i.e., – *tert*-butyl branches, benzene ring with more than two substituents and K_{ow} >3).

Since no experimental bioaccumulation data for DTBSBP were available, available analogue data and modelled log Kow, bioaccumulation factor (BAF) and bioconcentration factor (BCF) data were considered. The high modelled Kow value of DTBSBP (log K_{ow} = 6.1; KOWWIN v.1.67) indicates that uptake through the diet is expected to be an important route of bioaccumulation in fish. BAF and BCF values were predicted for DTBSBP and the two analogues using the Arnot-Gobas kinetic model corrected for metabolic rate for middle trophic level fish (BCFBAF, 2008, v.3.00). The BCF and BAF values predicted by this model for DTBSBP (BCF = 22 387 L/kg, BAF = 870 963 L/kg) and the two analogues (BCF = 3119 and 14 050 L/kg, BAF = 7534 and 324 700 L/kg for 2,6-di-*tert*-butyl-4-ethylphenol and 2,4,6-tri-*tert*-butylphenol respectively) indicate that DTBSBP is likely to be highly bioaccumulative. The Arnot-Gobas model was shown to be a good predictor of the empirical BCF data when compared with the available empirical fish BCF data for the analogue substances (highest BCF = 4870 to 5060 for 2,6-di-*tert*-butyl-4-ethylphenol, and BCF = 16 000 to 23 000 L/kg for 2,4,6-tri-*tert*-butylphenol). Therefore, more weight is given to the results of the Arnot-Gobas model than to the results of the other two BCF models employed (BCFBAF 2008 v.3.00 – without correction for metabolic rate, and Dimitrov model in the Canadian POPs Model suite 2008), which produced BCF values of less than 5000.

There are no experimental data available for the aquatic toxicity of DTBSBP, therefore modelled and analogue data were used to estimate the potential for aquatic toxicity. Toxicity values were predicted for DTBSBP in fish (96h LC50 = 0.039-0.1 mg/L; 60-day EC50 0.007 mg/L), water flea (96h EC50 0.015-0.93 mg/L; 21-day EC50 =0.12 mg/L), and algae (96h EC50 0.20 mg/L; chronic EC50 0.09 m/L) using the models ECOSAR 2008 v.1.00,

Canadian POPs Model 2008, AIEPS 2003-2007 v.2.05, and TOPKAT 2008 v.6.2. The lowest predicted aquatic toxicity value for DTBSBP is the 60-day chronic EC50 value of 0.007 for fish (ECOSAR, 2008, v.1.00). In ECOSAR, toxicity predictions for DTBSBP were modelled as a phenol rather than as a neutral organic. However, the predictions for DTBSBP modelled as a neutral organic are very similar to the ECOSAR values modelled as a phenol. All toxicity predictions appear to be within the applicability domains of the models as none of the maximum K_{ow} and molecular weight cut-off values specified in ECOSAR are exceeded. In addition, the predictions are below the estimated water solubility of the substance. The following empirical aquatic toxicity data for the analogue 2,4,6-tri-*tert*-butylphenol are available: fish (48-96 h LC50 0.06->10 mg/L), water flea (48h LC50 = 0.11 mg/L; 21-day reproduction NOEC 0.36 mg/L), and algae (72h NOEC =0.32 mg/L). The lowest measured analogue read-across aquatic toxicity value for 2,4,6-tri-*tert*-butylphenol is a 96-h LC50 of 0.06 mg/L for fathead minnow. The measured toxicity values seem to generally support the modelled toxicity values for DTBSBP.

DTBSBP possesses properties indicating a hazard for the environment (acute and chronic aquatic toxicity below 1 mg/L, not readily biodegradable and has high bioaccumulation potential).

Exposure Summary Information

DTBSBP is an organic substance that is used in Canada and elsewhere as an antioxidant and liquid stabilizer in plastics such as polyvinyl chloride (PVC) and polyurethane, as well as in brake fluids, ink resins and mineral/vegetable oils used industrial applications. It is also used as an antioxidant in the petrochemical sector.

This substance is not naturally produced in the environment. Currently the only known global manufacturer of this substance is located in the United States. A quantity of 16 686 kg of DTBSBP was imported into Canada in 2006, for use mainly in plastics manufacturing. The quantity of DTBSBP imported into Canada, along with the potentially dispersive uses of this substance, indicates that it may be released into the Canadian environment.