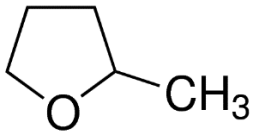
CAS Number: 96-47-9

QCAT Evaluation:
Author: Tony Cooper
Title: Chemical Engineer
Organization: WA State Dept. Ecology
Date: July 20, 2016

Peer Review:
Reviewer: Alex Stone
Title: Safer Chemical Alternative Chemist
Organization: WA Dept. of Ecology
Date: November 28, 2016

QCAT Chemical Assessment

Chemical Name:	**2-Methyltetrahydrofuran**
CAS #:	**96-47-9**
Also Called:	**Source: RTECS Database** **2-MeTHF, MTHF, Tetrahydro-2-methylfuran, Tetrahydrosylvan**
Identify Applications/ Functional Uses:	**Source: Wikipedia** 2-Methyltetrahydrofuran is mainly used as a higher boiling substitute for tetrahydrofuran as a specialty solvent. It also is used in the electrolyte formulation for secondary lithium electrodes and as a component in alternative fuels. It is a valued solvent for low temperature reactions. 2-Methyltetrahydrofuran forms a glass, which does not crystallize, and is frequently used as a solvent for spectroscopic studies at −196 °C. Other common uses of 2-methyltetrahydrofuran is as a solvent for Grignard reagents used in organometallic and biphasic chemical processes, because of the oxygen atom's ability to coordinate to the magnesium ion component of the Grignard reagent, or to azeotropically dry products. The use of 2-methyltetrahydrofuran provides very clean organic-water phase separations. It is a popular, but costlier substitute for tetrahydrofuran. 2-Methyltetrahydrofuran is approved by the United States Department of Energy as an additive to gasoline. 2-Methyltetrahydrofuran Furfural and other partially hydrogenated/reduced furyl compounds between it and 2-methyltetrahydrofuran (furfuryl alcohol, methylfuran, tetrahydrofural alcohol) have a tendency to polymerize and are quite volatile. 2-Methyltetrahydrofuran itself, however, is more stable and less volatile, and thus is suitable for use as a motor fuel. Source: Pubchem Methyltetrahydrofuran is a colorless liquid with an ether-like odor. Less dense than water. Vapors heavier than air. Used to make other chemicals and as a solvent.
Molecular Formula:	**$C_5H_{10}O$**
Molecular Weight:	**86.13**
Chemical Structure:	

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	2-Methyltetrahydrofuran has one chiral center, so it exists in two enantiomeric forms. The commercial processes involving hydrogenation gives a racemic mixture of the two. The asymmetric synthesis of (S)-(+)-2-methyltetrahydrofuran can achieved by using a wool–rhodium complex as a chiral catalyst for hydrogenation of methyl furan.
Optional Physicochemical Properties:	**Source: Wikipedia** 2-Methyltetrahydrofuran is "inversely soluble" in water. That is, its solubility decreases with increasing temperature, which is a rare property. 2-Methyltetrahydrofuran behaves like tetrahydrofuran as a Lewis base in organometallic reactions.

Hazard Summary Table:

Human Health Group 1 (HH1)					Human Health Group 2 (HH2)							Ecological			Fate		Physical	
C	M	R	D	E	AT	ST	N	SnS	SnR	IrS	IrE	AA	CA	E_o	P	B	Ex	F
DG	DG	DG	DG	DG	L							DG			M	vL		

Note: Please see Appendix A for glossary of hazard endpoint acronyms.

Grades		
Initial	**Data Gap**	**Final**
B	F	F_{dg}

Human Health Effects – Group I

Carcinogenicity (C) Hazard Level (H, M, L or DG): DG

- Research Summary: Due to the lack of Reproductive Toxicity data in Step I or II sources, 2-Methyltetrahydrofuran has a Development Toxicity Hazard Level of **DG**.

- References:

  No data available. ECHA C&L Inventory indicates “data lacking” for this Hazard Level.

Mutagenicity and Genotoxicity (M) Hazard Level (H, M, L or DG): DG

- Research Summary: Due to the lack of Mutagenicity and Genotoxicity data in Step I or II sources, 2-Methyltetrahydrofuran has a Development Toxicity Hazard Level of **DG**.

- References:

Little data available. No Step I sources available. The only Step II source with any information about mutagenicity and genotoxicity is the ECHA C&L Inventory. It indicates "conclusive but not sufficient for classification" for this Hazard Level.

Reproductive Toxicity (R) Hazard Level (H, M, L or DG): DG

- Research Summary: Due to the lack of Reproductive Toxicity data in Step I or II sources, 2-Methyltetrahydrofuran has a Development Toxicity Hazard Level of **DG**.

- References:

No data available. ECHA C&L Inventory indicates "data lacking" for this Hazard Level.

Development Toxicity incl. Developmental Neurotoxicity (D) Hazard Level (H, M, L or DG): DG

- Research Summary: Due to the lack of Development Toxicity data in Step I or II sources, 2-Methyltetrahydrofuran has a Development Toxicity Hazard Level of **DG**.

- References:

No data available. EC HA C&L Inventory indicates "data lacking" for this Hazard Level.

Endocrine Disruption (E) Hazard Level (H, M, L or DG): DG

- Research Summary: Due to the lack of Endocrine Disruption data in Step I or II sources, 2-Methyltetrahydrofuran has an Endocrine Disruption Hazard Level of **DG**.

- References:

No data available.

Human Health Effects – Group II

Acute Mammalian Toxicity (AT) Hazard Level (vH, H, M, L or DG): L

- Research Summary:

Pharos lists 2-Methyltetrahydrofuran on the New Zealand – GHS – 6.1E (inhalation) – acutely toxic and New Zealand – GHS – 6.1E (dermal) – acutely toxic. These listing both indicate a low (**L**) Acute Mammalian Toxicity Hazard Level. The ECHA C&L Inventory, a Step II source, lists 2-Methyltetrahydrofuran as Acute Tox. 4 (H302 – Harmful if swallowed) and Acute Tox. 4 (H332 – Harmful if inhaled), both of which indicate a moderate (**M**) Acute Mammalian Toxicity Hazard Level. RTECS, a Step II source, lists 2-Methyltetrahydrofuran dermal $LD_{50,rabbit}$ = 4500 mg/kg (**L**), Inhalation $LC_{50,rat}$ = 6000 ppm/4H (**M**) technical criteria.

While two Step II sources have more conservative Hazard Level data points, this QCAT will use the Step I source's conclusion of a low (**L**) Acute Mammalian Toxicity Hazard Level due to concerns raised in Ecology's QCAT Guidance document in Appendix 2 regarding ECHA C&L

data that "has not undergone review and there are some concerns about its accuracy." Moreover, the primary uses of the chemical are in its liquid state and thus less likely to be easily inhaled, mitigating some of the moderate hazard level end points.

- References:

  Step I sources:

  Pharos Project:

  New Zealand GHS – 6.1E (inhalation) – Acutely toxic; New Zealand GHS – 6.1E (dermal) – Acutely toxic

  Step II sources:

  ECHA C&L Inventory: Acute Tox. 4 (H302 – Harmful if swallowed); Acute Tox. 4 (H332 – Harmful if inhaled)

  RTECS: Dermal $LD_{50,rabbit}$ = 4500 mg/kg, Inhalation $LC_{50,rat}$ = 6000 ppm/4H

Environmental Health Effects

Acute Aquatic (AA) Toxicity Hazard Level: (vH, H, M, L or DG):

- Research Summary:

  There are no Step I sources available for Acute Aquatic Toxicity. The only Step II source with Acute Aquatic Toxicity data available is US EPA ECOTOX Database. There are two data points, but no endpoint (i.e., LC_{50}, EC_{50}) is reported for either. This indicates a Data Gap (**DG**) for Acute Aquatic Hazard Level.

  References:
  No data available.

Environmental Fate

Persistence (P) Hazard Level: (vH, H, M, L, vL or DG): M

- Research Summary: 2-Methyltetrahydrofuran has different Persistence Hazard Levels depending on the media of concern. Per US EPA PBT Profiler, 2-Methyltetrahydrofuran has a:

  - Half-life of 15 days in water, thus the Persistence Hazard Level is **L**.
  - Half-life of 30 days in soil, thus the Persistence Hazard Level is **M**.
  - Half-life of 0.75 days in air, the Persistence Hazard Level is **L**.
  - Half-life of 140 days in sediment, the Persistence Hazard Level is **H**.

However, because of the likelihood that the compound will be primarily found in soil (59%) and water (37%), the Persistence Hazard Level is assigned as **M**. If one were to have a specific example of the chemical in a different medium than soil, the **L** or **H** hazard level could be used accordingly.

- References:

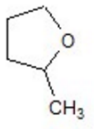
  PBT Profiler

Methodology · Criteria · Definitions · Chemicals That Should Not be Profiled
Home · Start a New Profile · Results · Terms of Use · Security

Results

Orange or red highlights indicate that the EPA criteria have been exceeded.
Black-and-white version

Persistence			Bioaccumulation	Toxicity
96-47-9 Furan, tetrahydro-2-methyl-				
PBT Profiler Estimate = PBT				
Media	**Half-Life (days)**	**Percent in Each Medium**	**BCF**	**Fish ChV (mg/l)**
Water	15	37%	3.6	24
Soil	30	59%		
Sediment	140	0%		
Air	0.75	3%		



P2 Considerations and more information.

Bioaccumulation (B) Potential Hazard Level: (vH, H, M, L, vL or DG): vL

- Research Summary: Based on information from US EPA PBT Profiler, 2-Methyltetrahydrofuran has a BCF of 3.6, and thus has a Bioaccumulation Potential Hazard Level of **vL**.

- References:

  PBT Profiler

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Results

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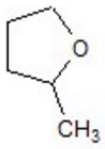
Black-and-white version

Persistence | Bioaccumulation | Toxicity

96-47-9 Furan, tetrahydro-2-methyl-

PBT Profiler Estimate = PBT

Media	Half-Life (days)	Percent in Each Medium	BCF	Fish ChV (mg/l)
Water	15	37%	3.6	24
Soil	30	59%		
Sediment	140	0%		
Air	0.75	3%		



P2 Considerations and more information .