

# Green Chemistry



Supporting the Advancement of Chemistry through Sound Environmental, Social and Fiscal Responsibilities



## ***Alternative Solvents***

Increased Safety, Low Peroxides Formation  
Reduced Environmental Footprint

- 2-Methyltetrahydrofuran
- Cyclopentyl methyl ether

## Green Chemistry

The aim of green chemistry is to reduce chemical related impact on human health and virtually eliminate contamination of the environment through dedicated, sustainable prevention programs. Green chemistry searches for alternative, environmentally friendly reaction media and at the same time strives to increase reaction rates and lower reaction temperatures.

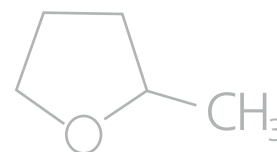
The green chemistry concept applies innovative scientific solutions to solve environmental issues posed in the laboratory. Paul T. Anastas, an organic chemist working in the Office of Pollution Prevention and Toxins at the EPA, and John C. Warner developed the **Twelve Principles of Green Chemistry** in 1991. These principles can be grouped into **Reducing Risk** and **Minimizing the Environmental Footprint**.

## 2-Methyltetrahydrofuran (2-MeTHF)

CAS No.: 96-47-9

### A Truly Green Alternative to Dichloromethane and Tetrahydrofuran

2-MeTHF is derived from **renewable resources** such as corncobs and bagasse. When used as an organometallic solvent, 2-MeTHF offers both economical and environmentally friendly advantages over Tetrahydrofuran.



### Features & Benefits

- Lower peroxide formation than THF (stabilizer required)
- Aprotic polar solvent
  - Resembles Toluene in physical properties
  - Grignard reagents tend to be more soluble in 2-MeTHF than in THF
- Forms an azeotrope rich with water
  - Can be **more easily dried** than THF or DCM
- Limited miscibility in water (4.1g/100g at 23°C)
  - Easy separation and recovery from water **reduces the waste stream**
- Higher boiling point (80°C) compared to THF
  - Higher reaction temperature **reduces overall reaction time**
- Low heat vaporization
  - **Less solvent loss** during reaction reflux
  - **Saves energy** during distillation and recovery

### Alternative to Tetrahydrofuran for Organometallic Reactions

- Grignard
- Reformatskii (Reformatsky)
- Lithiation
- Hydride Reduction
- Metal-Catalyzed Coupling (Heck, Stille, Suzuki)

### Alternative to Dichloromethane for Biphasic Reactions

- Alkylation
- Amidation
- Nucleophilic Substitution Reaction

2-Methyltetrahydrofuran	Cat. No.
Anhydrous, ≥99.0%	414247-100ML
Contains 250 ppm BHT	414247-1L
	414247-6X1L
	414247-2L
	414247-4X2L
	414247-200L-P2
Anhydrous, ≥99.0%	673277-100ML
Inhibitor-free	673277-12X100L
	673277-1L
	673277-200L-P2
ReagentPlus®, ≥99.5%	155810-100ML
Contains 150-400 ppm BHT	155810-12X100ML
	155810-500ML
	155810-4X4L
	155810-20L



Looking to reduce the number of glass bottles in your lab? For more information on our Returnable Containers Program, please visit us at [sigma-aldrich.com/rc](http://sigma-aldrich.com/rc).



## The Sigma-Aldrich Global Commitment

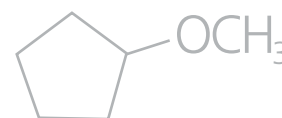
Sigma-Aldrich has a proud tradition of sound environmental, social and fiscal responsibility. We are committed to sustainable growth which is good for the environment, our people, and our customers.

## Cyclopentyl methyl ether (CPME)

CAS No.: 5614-37-9

### Environmentally Friendly Alternative to Tetrahydrofuran, tert-Butyl methyl ether (MTBE), 1,4 Dioxane and other ether solvents

CPME provides a green solution for those looking to improve their chemical process by not only minimizing the solvent waste stream, but also improves laboratory safety due to CPME's unique composition which resists the formation of peroxides.



### Features & Benefits

- More stable than THF and 2-MeTHF (stabilizer required)
  - **Resists peroxide formation**
  - **Reduces** the frequency of peroxide testing
- Novel hydrophobic ether solvent
  - Useful in many organometallic reactions
  - **Provides better yields** and higher selectivity over THF
- Forms an azeotrope rich with water
  - Can be more **easily dried** than THF and 2-MeTHF
- Limited miscibility in water (1.1g/100g at 23°C)
  - Easy separation and recovery from water **reduces the waste stream**
- Higher boiling point (106°C) compared to THF and 2-MeTHF
  - Higher reaction temperature **reduces overall reaction time**
- Low heat vaporization
  - **Less solvent loss** during reaction reflux
  - **Saves energy** during distillation and recovery

### CPME Applications

#### Higher Optical Purity or Selectivity were Observed

- Asymmetric Michael Alkylation
- Michael addition of  $R_2CuLi$
- Alkylation of chiral amide
- Glycosidation
- Asymmetric hydrogenation of  $NaBH_4$
- Hydrosilylation by Ru cat

#### Nucleophilic Reactions

- Amide synthesis by the reaction of acid chloride with amine
- Silylation and desilylation
- Reaction of Carbon anion with aldehyde
- Debenzylation
- Alkylation of amine
- Selective methylation of phenols
- Bromination of alcohol with  $PBr_3$
- Sulfonylchloride synthesis by the reaction of sulfonic acid with  $PCl_5$

#### Reactions using Metals

- Reaction of ketone using  $NaBH_4$
- Reaction of acetylenes with  $Ti(OR)_4$
- Reaction using n-BuLi or Lithium Diisopropyl Amide
- Radical cyclization of trichloroacetate using Cu cat
- Reduction of ethyl benzoate using Lithium Aluminium Hydride
- Formation of sodium dispersion
- Intramolecular ene reaction using  $ZnCl_2$

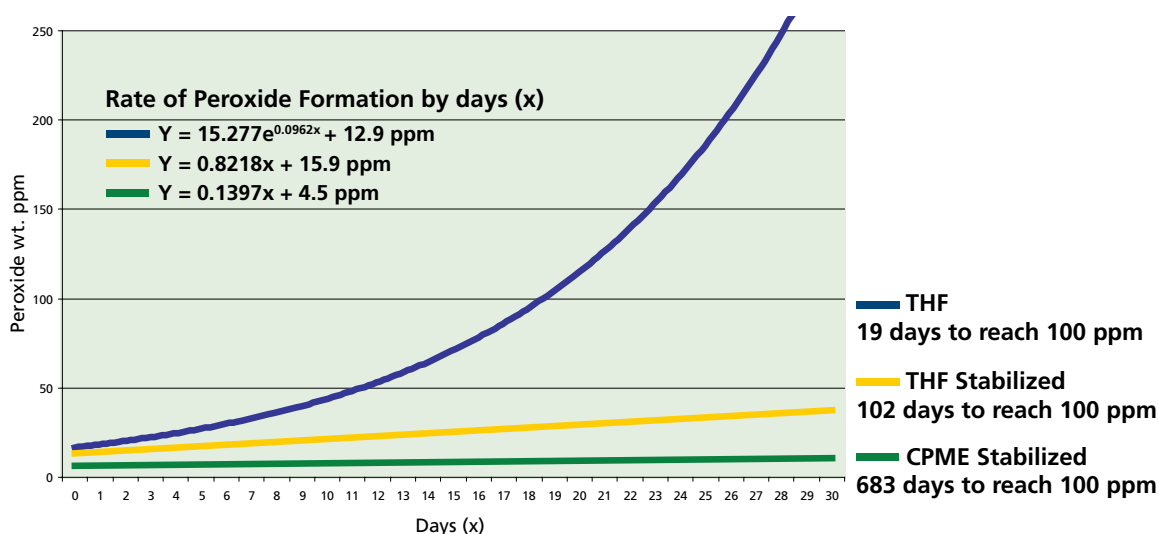
Cyclopentyl methyl ether	Cat. No.
Anhydrous, $\geq 99.9\%$ Contains 50 ppm BHT	<a href="#">675970-100ML</a> <a href="#">675970-1L</a> <a href="#">675970-2L</a>
ReagentPlus®, $\geq 99.9\%$ Contains 50 ppm BHT	<a href="#">675989-500ML</a> <a href="#">675989-1L</a> <a href="#">675989-4L</a>

CPME is a proven alternative to THF, providing **better yields** and **higher selectivity**.

## Physical Properties of Solvents

Properties	CPME	2-MeTHF	THF	Ether	DCM	1,4-Dioxane	MTBE
Density (20 °C) [g/cm <sup>3</sup> ]	0.86	0.86	0.89	0.71	1.32	1.03	0.74
Dielectric constant (25 °C)	4.76	6.97	7.58	4.197	8.93	2.227	—
Boiling point [°C]	106	80	65	34.6	39.8	101	55
Heat of Vaporization (bp) [Kcal/kg]	69.2	87.1	98.1	86.1	80.5	98.6	81.7
Solubility of Solvent in Water (23 °C)	1.1	14	Infinite	6.5	1.3	Infinite	4.8
Solubility of Water in Solvent (23 °C)	0.3	4.4	Infinite	1.2	0.2	Infinite	1.5
Azeotropic temperature with Water [°C]	83	89	64	34	39	88	52
Flash point [°C]	-1	-11.1	-14.2	-45	—	12	-28
Explosion range [vol%] Lower / Upper limit	1.1% / 9.9%	—	1.84% / 11.8%	1.85% / 48%	14% / 22%	2% / 22%	1.6% / 15.1%

## Peroxide Formation of Ether Solvent



### Conditions

- 20 mL of each sample in a brown bottle (capacity of 65 mL)
- Stored at room temperature, in a dark place and in the presence of air

CPME is a product of Zeon Corporation with approval by Toxic Substances Control Act (TSCA) and European List of Notified Chemical Substances (ELINCS).

Check out the new  
**Spec Comparison** page  
 to find the perfect Sigma-Aldrich  
 solvent for your application.  
[sigma-aldrich.com/solvents](http://sigma-aldrich.com/solvents)

### World Headquarters

3050 Spruce St., St. Louis, MO 63103  
 (314) 771-5765  
[sigma-aldrich.com](http://sigma-aldrich.com)

**Order/Customer Service** (800) 325-3010 • Fax (800) 325-5052

**Technical Service** (800) 325-5832 • [sigma-aldrich.com/techservice](http://sigma-aldrich.com/techservice)

**Development/Bulk Manufacturing Inquiries SAFC™** (800) 244-1173

©2007 Sigma-Aldrich Co. All rights reserved. SIGMA, SAFC, SAFC, SIGMA-ALDRICH, ALDRICH, FLUKA, and SUPELCO are trademarks belonging to Sigma-Aldrich Co. and its affiliate Sigma-Aldrich Biotechnology, L.P. Sigma brand products are sold through Sigma-Aldrich, Inc. Sigma-Aldrich, Inc. warrants that its products conform to the information contained in this and other Sigma-Aldrich publications. Purchaser must determine the suitability of the product(s) for their particular use. Additional terms and conditions may apply. Please see reverse side of the invoice or packing slip.

03704  
0107



Printed on Recycled Paper —  
 A Worldwide Operation with a Global Commitment