Greener
Solvent Alternatives

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

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.

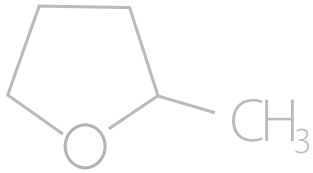
The green chemistry concept applies innovative scientific solutions to solve environmental issues posed in the laboratory. Paul T. Anastas, an organic chemist working in the Office of Pollution Prevention and Toxins at the EPA, and John C. Warner developed the Twelve Principles of Green Chemistry in 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
  - Bromo and Iodo Grignards tend to be more soluble in 2-MeTHF where as chloro Grignard reagents tend to be less soluble
- Forms an azeotrope rich with water
  - Can be more easily dried than THF or DCM
- Limited miscibility in water (14g/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 refl ux
  - 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

Cat. No.	2-Methyltetrahydrofuran
414247-100mL 414247-1L 414247-6x1L 414247-2L 414247-4x2L 414247-200L-P2	Anhydrous, ≥99.0% Contains 250 ppm BHT
673277-100mL 673277-12x100mL 673277-1L 673277-200L-P2	Anhydrous, ≥99.0% Inhibitor-free
155810-100mL 155810-12x100mL 155810-500mL 155810-4x4L 155810-20L	*ReagentPlus*®, ≥99.5% Contains 150-400 ppm BHT

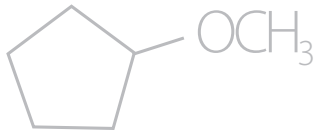
Looking to reduce the number of glass bottles in your lab? For more information on our Returnable Containers Program, visit us at **sigma-aldrich.com/rc**

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
- Sillylation and desillylation
- 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 $ZnCl_2$

Cat. No.	Cyclopentyl methyl ether
675970-100mL 675970-1L 675970-2L	Anhydrous, ≥99.0% Contains 50 ppm BHT
675989-500mL 675989-1L 675989-4L	*ReagentPlus*®, ≥99.9% Contains 50 ppm BHT

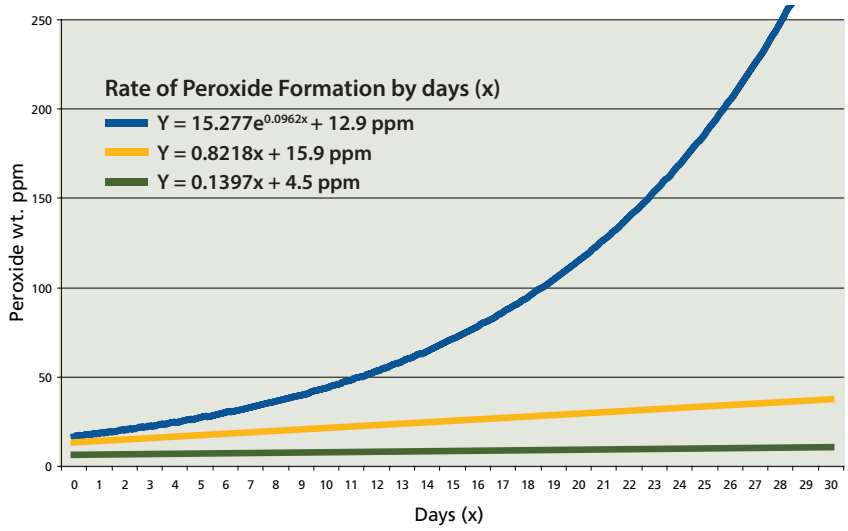
CPME is a proven alternative to THF, providing better yields and higher selectivity.

Check out the new Spec Comparison page to find the perfect Sigma-Aldrich solvent for your application.
sigma-aldrich.com/solvents

Physical Properties of Solvents

Properties	CPME	2-MeTHF	THF	Ether	DCM	1,4-Dioxane	MTBE
Density (20 °C) [g/cm3]	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



THF 19 days to reach 100 ppm

THF Stabilized 102 days to reach 100 ppm

CPME Stabilized 683 days to reach 100 ppm

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).

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