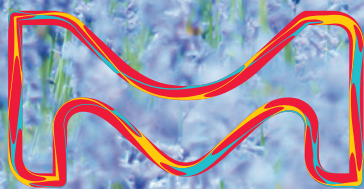


MERCK

THE FUTURE
OF SOLVENTS:

BIO
RENEWABLE



The life science
business of Merck
operates as
MilliporeSigma in
the U.S. and Canada.

Sigma-Aldrich®
Lab & Production Materials



Dedicated to supporting all your explorations

RESPONSIBLY.

Why should you have to choose between solvents that are ecological and those that are reliable? Enjoy both at once with our biorenewable and greener solutions. Thanks to their origin, they won't compromise the environment. And thanks to their high quality, they won't compromise your work.

In addition to our familiar greener solvents, such as water and ethanol, you also have the option of other innovative solutions that are made from biological sources, have higher recovery rates, or are safer for handling and disposal. Many of them are based on non-food, biorenewable materials, so they don't depend on petroleum sources, or deplete food supplies. Certain solvents are still essential for scientific work.

But, here too, we're investing in promising research to find optimal, safer alternatives for you. Explore our latest range of greener and biorenewable solvents, and see how your explorations go even further through sustainability.



Learn more about our dedication
to green chemistry on:
SigmaAldrich.com/greener

The 12 principles of green chemistry

In 1998, Paul Anastas and John Warner proposed a framework to change how scientists thought about their work by making environmentally friendly chemical processes and products top of mind.

Their 12 principles are represented by the icons below, which provide a **quick reference for the classification of our greener substitutes and biorenewable solvents.**



Use of Renewable Feedstocks



Safer Solvents and Auxiliaries



Design for Degradation



Prevention of Waste



Designing Safer Chemicals



Inherently Safer Chemistry for Accident Prevention



Design for Energy Efficiency



Reduced Derivates



Catalysis



Atom Economy



Less Hazardous Chemical Syntheses



Real-Time Analysis for Pollution Prevention



Explore our complete range of solvents on:
[SigmaAldrich.com/solvents](https://www.sigmaaldrich.com/solvents)



Biorenewable solvents. A simple switch.

It's now easy for everyone – from the smallest universities to the largest pharmaceutical and technology companies – to implement greener chemistry. Simply replace classic petroleum solvents in your current workflows with our biorenewable alternatives and proceed as you always have.

These solvents are free of the many by-products of petroleum manufacturing, such as benzene, aldehydes, and ethers. What's more, each solvent is verified as renewable through ASTM testing (ASTM Standard D6866-16), which verifies the percentage of new carbon.

Acetone (904082)			
Property Tested	Renewable Acetone	Non-Renewable Acetone	Test Method
Total purity	≥ 99.5%	≥ 99.5%	GC
Water	≤ 0.3%	≤ 0.5%	ASTM D1364
Benzene	Not Detected	0.003%	GC
Aldehydes	Not Detected	≤ 0.002%	GC
Methanol	≤ 0.05%	≤ 0.05%	GC
Isopropanol	≤ 0.05%	≤ 0.05%	GC
Nonvolatile Matter wt%	≤ 1 mg / 100 mL	≤ 0.001%	ASTM D1353
Renewable Carbon wt%	100%	0%	ASTM D6866

1-Butanol (901351)			
Property Tested	Renewable 1-Butanol	Non-Renewable Butanol	Test Method
Total purity	≥ 99.8%	≥ 99.4%	GC
Di-n-butyl ether	Not detected	≤ 0.2%	GC
Isobutanol	Not Detected	≤ 0.1%	GC
Aldehydes	Not Detected	≤ 0.01%	GC
Water	≤ 0.05%	≤ 0.1%	ASTM D1364
Nonvolatile Matter wt%	≤ 1 mg / 100 mL	≤ 0.005%	ASTM D1353
Renewable Carbon wt%	100%	0%	ASTM D6866

Cat. No.	Product Description
901351	1-Butanol, Biorenewable, ACS Reagent, ≥ 99.4%
904082	Acetone, Biorenewable, ACS Reagent, ≥ 99.5%

It may seem like a small change but by choosing a greener alternative you are joining thousands of scientists who are designing a new future that uses resources more responsibly. One small change early on has the potential to help make the world better for the generations to come.

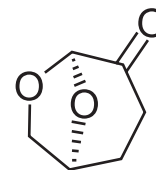
Join us in taking giant steps toward creating smaller footprints. To find out more visit [SigmaAldrich.com/cr](https://www.sigmaaldrich.com/cr)



Cyrene™

CAS No.: 53716-82-8

Alternative for: NMP, DMF, and sulfolane



Features & benefits

Cyrene™ is a new dipolar aprotic alternative to common REACH-restricted solvents, such as N-methyl-2-pyrrolidone (NMP). One of the first true greener solvents, it is produced from renewable resources, and safe for end of life disposal, decomposing into CO₂ and H₂O. Cyrene™ is also safer to handle, with no mutagenic or genotoxic concerns.

- 99% biodegradation in 28 days
- Stable during incineration
- Not mutagenic or genotoxic

Applications:

- Exceeds NMP's dispersive ability for graphene solutions by an order of magnitude¹
- Used as an alternative to DMF in synthesis of metal-organic frameworks²
- Comparable replacement for DMF in amide and dipeptide coupling reactions³

Reactions:

- Sonogashira
- Cacchi-type annulation
- Synthesis of metal-organic frameworks
- Suzuki-Miyaura coupling reaction
- Synthesis of ureas

Cat. No.	Product Description
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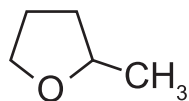
807796	Cyrene™
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- ¹ Identification of high performance solvents for the sustainable processing of graphene, Salavagoine, H., Sherwood, J., De bruyn, M., Budarin, V., Ellis, G., Clark, J., Shuttleworth, P., Green Chem, 2017, 11, 2550-2560
- ² Dihydrolevoglucosenone (Cyrene) as a Green Alternative to N,N-Dimethylformamide (DMF) in MOF Synthesis, Zhang, J., White, G., Ryha, M., Hunt, A., Katz, J., ACS Sustainable Chem Eng., 2016, 4(12), 7186-7192
- ³ Cyrene as a bio-based solvent for HATU mediated amide coupling, Wilson, K., Murray, J., Jamieson, C., Watson, A., Org Biol. Chem, 2018, 16, 2851-2854

2-Methyltetrahydrofuran (2-MeTHF)

CAS No.: 96-47-9

Alternative for: THF, diethyl ether, and DCM



Features & benefits

2-Methyltetrahydrofuran is an environmentally favorable alternative to tetrahydrofuran (THF), 1,4 dioxane (dioxane), and dichloromethane (DCM) for most industrial applications.

- High boiling point: Processes may be run at higher temperatures, decreasing reaction time
- Organic water-phase separation: Limits need for extraction solvents, lowers solvent and water waste
- Reduced energy to recover: Standard distillation is sufficient for solvent recovery
- No risk of genotoxicity or mutagenicity from exposure

Other applications:

Forms organic (non-crystalline) glass for low temperature (-196°C) spectroscopic studies

Alternative for THF in organometallic reactions:

- Grignard
- Reformatsky
- Lithiation
- Hydride reduction
- Metal-catalyzed coupling (Heck, Stille, Suzuki)

Alternative for dichloromethane in biphasic reactions:

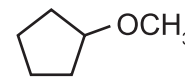
- Alkylation
- Amidation
- Nucleophilic substitution

Cat. No.	Product Description
155810	ReagentPlus®, ≥ 99.5%, contains 150-400 ppm BHT as stabilizer
414247	Anhydrous, ≥ 99.0%, contains 250 ppm BHT as stabilizer
673277	Anhydrous, ≥ 99%, inhibitor-free
900520	Anhydrous, contains 250 ppm BHT as stabilizer, ZerO ₂ ®, ≥ 99.0%

Cyclopentyl methyl ether (CPME)

CAS No.: 5614-37-9

Alternative for: THF, t-butyl methyl ether (MTBE), dioxane, and other ether solvents



Features & benefits

Cyclopentyl methyl ether (CPME) is a hydrophobic ether solvent with a high boiling point, making it an optimal substitute for many ether solvents, such as MTBE and THF. CPME is made of renewable resources, and offers other benefits, including significantly safer handling.

- Low peroxide formation⁴
- High hydrophobicity⁴
- High boiling point, low melting point⁴
- Narrow explosion area⁴

Applications:

- Crystallization⁵
- Polymerization
- Coatings

Reactions:

- Alkali agent (nucleophilic substitution of heteroatoms)
- Azeotropic removal of water
- Transition metal catalysis
- Organometallic
- Lewis acid mediated reactions

Cat. No.	Product Description
675989	CPME, contains 50 ppm BHT as inhibitor, ReagentPlus®, ≥ 99.9%
675970	CPME, contains 50 ppm BHT as inhibitor, anhydrous, ≥ 99.9%
791962	CPME, inhibitor-free, anhydrous, ≥ 99.9%


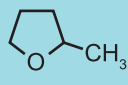
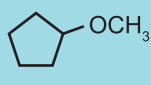
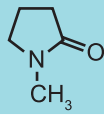
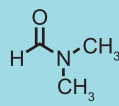



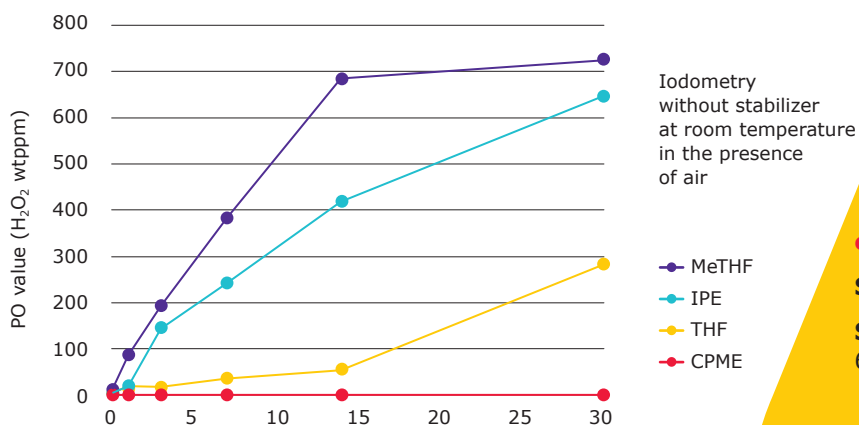
Looking to further reduce your environmental impact?

Explore more green solvent alternatives on: SigmaAldrich.com/greensolvents

4 The toxicological assessment of cyclopentyl methyl ether (CPME) as a green solvent. Watanabe, K., Molecules 2013, 18(3), 3183-94
5 Cyclopentyl Methyl Ether: An Elective Eco-Friendly Etheral Solvent in Classical and Modern Organic Chemistry, Azena, U., Carraro, M., Pisano, L., Monticelli, S., Barolotta, R., Pace, V., Chem Sus. 2018

Greener alternative solvents at a glance

Solvent	THF	MeTHF	CPME	NMP	DMF	Cyrene
Structure						
CAS No.	109-99-9	96-47-9	5614-37-9	872-50-4	68-12-2	53716-82-8
Density (g/mL)	0.928	0.85	0.86	1.028	0.994	1.250
Boiling Point (°C)	65.8	80	106	204	153	116
Melting Point (°C)	-108	-136	< -140	-24	-61	< -20
Dielectric Constant	7.58	7	4.76	32.2	38.25	~3.4
Dipole Moment (D)	1.7	1.38	1.27	12.26	3.8	Unknown
Solubility in Water (mol/L)	13.9	14	0.226	10.1	13.7	∞
Viscosity (cP)	0.589	0.6	0.55	1.65	0.805	14.5
Surface Tension (dyn/cm)	27.4	25.9	25.17	40.79	37.10	72.5
Vaporization Energy (kJ/mol)	98.1	89.7	69.2	61.9	47.6	Unknown
Flash Point (°C)	-14.5	-11	-1	91	58	108
Ignition point (°C)	205	270	180	245	445	296
Catalog No.	360589 676764 186562 401757	155810 414247 673277 900520	675989 675970 791962	443778 328634	437573 319937 227056	807796



Iodometry without stabilizer at room temperature in the presence of air

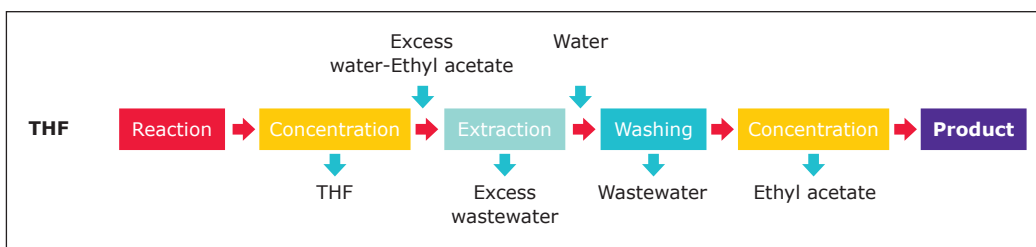
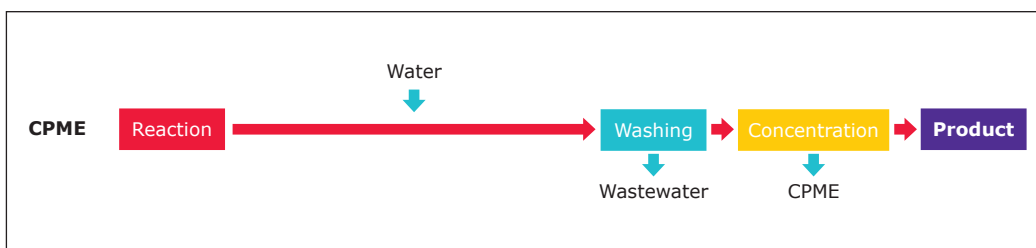
Peroxide formation comparison of MeTHF, isopropyl ether (IPE), THF, and CPME over 25 days.

Stabilized THF: 102 days to reach 100ppm

Stabilized CPME:

683 days to reach 100 ppm

The product is stabilized with approximate 50 ppm of BHT



CPME vs. THF process flow.

CPME reduces the number of steps required for production. It reduces the amount of water that is required for washing and eliminates the need for co-solvents for product recovery.

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Lab & Production Materials

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