Sustainable Chemistry

Green Solvents - Safety - Quality

DASITGROUP | CARLO ERBA REAGENTS

Sustainable Chemistry

The growing awareness of the environmental impact of chemical products and the process used to produce them has led to the development of the concept of "Green Chemistry".

In 1991, Paul T. Anastas, working at the EPA, and John C. Warner developed the **Twelve Principles of Green Chemistry.**[1] These principles are best described by the definition given by their founders : "*Green chemistry is the utilization of a set of principles that reduces or eliminates the use and generation of hazardous substances in the design, manufacture and application of chemical products.*"

CARLO ERBA Reagents has been an active actor driving the development and adoption of "green chemistry". We strive to minimize the ecological impact of chemistry by not only offering a wide array of **green solvents** but also services such as **returnable containers**.

[1] Anastas, P. and Warner, J. C., *Green Chemistry: Theory and Practice* **1998**

Green solvents

Besides the obvious "green solvents", water and ethanol, CARLO ERBA Reagents is happy to offer a variety of greener alternatives to several common solvents :

- 2-Methyltetrahydrofuran (2-MeTHF)
- 4-Methyltetrahydropyran (MTHP)
- Cyclopenthylmethylether (CPME)
- n,n'-Dimethylpropyleneurea (DMPU)
- 1,3-Propanediol
- 1,3-Dioxolane

Equivalency table :

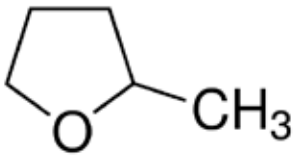
	Dichloro-methane (DCM)	Tetrahy-drofuran (THF)	Dimethyl-sulfoxide (DMSO)	Dimethyl-formamide (DMF)	tert-Butyl-methyl ether (MTBE)	Dioxane	Diethyl ether	Toluene	Xylene
2-MeTHF									
CPME									
DMPU									
MTHP									
1,3-Dioxolane									

These greener alternatives have the following characteristics vs. those of some common solvents :

	CAS	MW (g/mol)	d 20°c (g/cm³)	BP [°C]	MP [°C]	FP [°C]	Viscosity (20°C) [cP]	Re-fractive index (20°C)	Dielec-tric con-stant (25°C)	Solu-bility in water (23°C) [g/100g]	Water solubility in the solvent (23°C) [g/100g]	Azeo-tropic point with water [°C]	Explo-sion range [vol%] (lower limit)	Explo-sion range [vol%] (upper limit)
MeTHF	96-47-9	86,14	0,85	80	-136	-11	0,6 (25°C)	1,41	7	14	4,4	71	1,5	8,9
1,3-propanediol	504-63-2	76,1	1,05	214	-26,7	129	0,52	1,44	—	∞	∞	—	2,6	16,6
CPME	5614-37-9	100,16	0.86	106	<-140		0.55	1.42	4.76	1.1	0.3	83(*)	1.1	9.9
DMPU	7226-23-5	128,18	1,06	246	-23	120	—	—	—	—	—	—	—	—
Dioxolane	646-06-0	74,08	1,07	75,6	-95	-6	0,6 (25°C)	1,40	7,34	∞	∞	71 (*)	2,1	20,5
MTHP	4717-96-8	100,16	0,86	105	-70	6,5	0,78	—	—	1,5	1,4	84,5	—	—
DMF	68-12-2	73,10	0,95	153	-61	58	0,80	1,42	—	∞	∞	—	2,2	16
NMP	872-50-4	99,13	1,03	202	-24	93	1,65	1,47	—	∞	∞	—	1,3	9,5
MEK	78-93-3	72,11	0,81	79,6	-86	-5	0,39	1,38	18	22,6	9,9		1,8	11,5
THF	109-99-9	72,11	0.89	65	-108.5	-14.5	0.55	1.41	7.58	∞	∞	64	1.84	11.8
Diethylether	60-29-7	74,12	0.71	34.6	-116.3	-45	0.245	1.35	4.20	6.5	1.2	34.2	1.85	48
Dioxane	123-91-1	88,11	1.03	101	11.8	12	1.31	1.42	2.23	∞	∞	87.8	2	22
MTBE	1634-04-4	88,15	0.74	55	-108.7	-28	—	1.37	—	4.8	1.5	—	1.6	15.1
Dichloromethane	75-09-2	84,93	1,32	39,6	-97	—	0,43	1,42	11	1,32	0,14	—	13	22

2-Methyltetrahydrofuran (2-MeTHF)

A truly green alternative to THF and DCM



CAS 96-47-9
MW 86,14 g/mol
Formula $C_5H_{10}O$
BP 80 °C

It is derived from **renewable sources** and guarantees superior versatility, efficiency and reactivity in Grignard and other organometallic reactions.[1] It is an **aprotic** solvent, not miscible in water and particularly suited for reactions in biphasic environments, such as alkylation amidation and nucleophilic substitutions.[2]

Advantages of 2-MeTHF over THF

- Higher boiling point (80 °C)
- Lower miscibility in water
- Produced from renewable sources
- Non-irritant to the eyes and respiratory tract
- Lower peroxide formation
- Better solubility for Grignard reagents
- Azeotrope with 10.6% of water

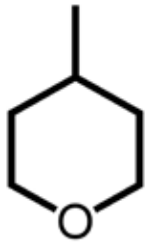
2-MeTHF is available in quality for synthesis and HPLC grade :

Description	Quality	Pkg	Code
2-Methyltetrahydrofuran	RE - Puro	1l	P9960216
2-Methyltetrahydrofuran	RE - Puro	2.5l	P9960221
2-Methyltetrahydrofuran	RE - Puro	5l	P9960229
2-Methyltetrahydrofuran	RE - Puro	25l	P9960248
2-Methyltetrahydrofuran	RE - Puro	200l	P9960268
2-Methyltetrahydrofuran	RS - HPLC Isocratic	1l	412681
2-Methyltetrahydrofuran	RS - HPLC Isocratic	2.5l	412682

1. Silverman, G. S. and Rakita, P., *Handbook of Grignard Reagents*, Marcel Dekker, **1996**.
2. Ripin, D. and Vetellno, M., *Synlett* **2003,** 15, 2353.

4-Methyltetrahydropyran (MTHP)

An innovative alternative to THF



CAS 4717-96-8
MW 100.16 g/mol
Formula $C_6H_{12}O$
BP 105 °C

This new hydrophobic cyclic ether is an excellent substitute to THF or 2-MeTHF in various applications (Grignard reactions, LAH reduction, cross coupling, etc...).

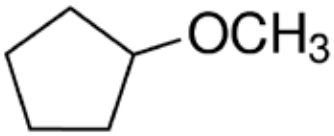
CARLO ERBA Reagents is introducing MTHP in quality "RE - Pure for synthesis" stabilized with BHT, suitable for all organic synthesis procedures.

Description	Quality	Pkg	Code
4-Methyltetrahydropyran	RE - Puro	500 ml	P9990218
4-Methyltetrahydropyran	RE - Puro	1l	P9990216
4-Methyltetrahydropyran	RE - Puro	2.5l	P9990221

For more information on applications, visit our website

Cyclopentyl methyl ether (CPME)

An attractive solvent



CAS	5614-37-9
MW	100.16g/mol
Formula	$C_6H_{12}O$
BP	105 °C

The **unique physical and chemical characteristic** of CPME makes it a great "green" alternative to the use of more common solvents such as THF, MTBE, 1,4 dioxane and other ether solvents. This solvent reduces the **amount of waste water** and other solvents due to its hydrophobicity, facilitating the extraction of the product. CPME has a high boiling point and a high stability with a lower formation of peroxide compare to analogous solvents. It is also stable under acidic and basic conditions.[1] It can be used for various reactions such as Grignard,[2] enolate formation,[1] or Pd based transformations.[3]

Advantages of CPME over other ethers

- Greater stability in acidic and basic environments
- Higher boiling point
- Limited solubility in water
- Low volatility
- Lower peroxide formation

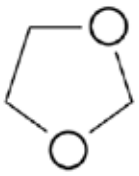
CPME is available in quality for synthesis grade :

Description	Quality	Pkg	Code
Cyclopentyl methyl ether	RE - Puro	1l	P8010216
Cyclopentyl methyl ether	RE - Puro	5l	P8010229
Cyclopentyl methyl ether	RE - Puro	25l	P8010248

1. Watanabe, K. et al. *Org. Process. Res. Rev.* **2007**, 11, 251
2. Kobayashi, S. et al. Asian *J. Org. Chem.* **2016**, 5, 636
3. Mao, J. et al. *Org. Lett.* **2014**, 16, 5304.

1,3-Dioxolane

An environmentally friendly solvent



CAS	646-06-0
MW	74.08g/mol
Formula	$C_3H_6O_2$
BP	75.6 °C

1,3-Dioxolane is an **odorless, non-toxic** and environmentally friendly solvent. Its physical, chemical and toxicological properties allow it to be used as a solvent or a reagent. It can not only be used as an alternative to dichloromethane, dichloroethane and methyl ethyl ketone under neutral or basic reaction conditions, but also in place of THF and DMSO. It is mostly used in the polymer industry as a solvent or as an inhibitor. It can also be used in organometallic and inorganic systems, lithium batteries or metal working and electroplating.[1]

Advantages over other solvents :

- Improved safety (not carcinogenic, toxic or explosive)
- More convenient to use (odorless)
- Low peroxide formation
- Miscible in water and most organic solvents

1,3-Dioxolane is available in quality for synthesis grade :

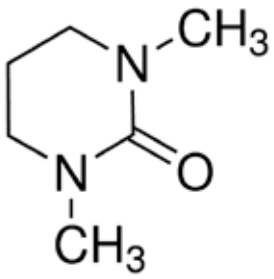
Description	Quality	Pkg	Code
1,3-Dioxolane	RE - Puro	1l	P8030216
1,3-Dioxolane	RE - Puro	5l	P8030222
1,3-Dioxolane	RE - Puro	25l	P8030249
1,3-Dioxolane	RE - Puro	200l	P8030268

1. http://www.intermediates.basf.com/chemicals/web/en/function/conversions:/publish/content/news-and-publications/brochures/download/BASF_Brochure_Dioxolane.pdf

n,n'-Dimethylpropylene urea (DMPU)

The best "greener" alternative for dipolar aprotic solvents

DMPU is an urea derived solvent, considered one of the best "greener" alternative for dipolar aprotic solvents due to its **reduced toxicity**.[1] Its particular physical and chemical properties, helping the activation of nucleophiles, make it a **solvent of choice for SN_2 reactions**.[2] It has shown to be a very valuable solvent in the synthesis of high value APIs where traditional processes are not delivering the expected results. This solvent can not be used in the pharmaceutical, agrochemical and electronic industry. It is an excellent substitute to HMPT, a carcinogenic product, used in the alkylation of lithium alkinides, key intermediate in the synthesis of pheromones.[3]



CAS	7226-23-5
MW	128.18g/mol
Formula	$C_6H_{12}N_2O$
BP	246 °C

Advantages :

- Less aggressive reaction medium
- Increase in yields
- Safer to handle

DMPU is available in quality for synthesis grade :

Description	Quality	Pkg	Code
n,n'-Dimethylpropylene urea	RE - Puro	500 ml	P8020218
n,n'-Dimethylpropylene urea	RE - Puro	1l	P8020216
n,n'-Dimethylpropylene urea	RE - Puro	5l	P8020229
n,n'-Dimethylpropylene urea	RE - Puro	25l	P8020248
n,n'-Dimethylpropylene urea	RE - Puro	200l	P8020268

1. Byrne, F. P. et al. *Sustain. Chem. Process* **2016**, 4.
2. Doolittle, R. E. *Org. Prep. Proced. Int.* **1980**, *12*, 1.
3. Lo, C.-C. et al. *J. Chem. Ecology* **1990**, *16*, 3245.

1,3-Propanediol

A solvent from renewable source

1,3-Propanediol is a product obtained from a renewable source, corn, with characteristics and performance comparable to petroleum derivative solvents.

It is biodegradable with a low toxicity and a greater thermal stability compared to other glycols and ethylene glycols. It is widely used in the manufacturing of polyester resins, urethane chemistry as well as the production of antifreeze and heat transfer fluids.

CAS	504-63-2
MW	76.09g/mol
Formula	$C_3H_8O_2$
BP	214 °C

Advantages :

- Low toxicity and biodegradability
- Good thermal stability
- Reduced environmental impact

1,3-Propanediol is available in quality for synthesis grade :

Description	Quality	Pkg	Code
1,3-Propanediol	RE - Puro	1l	P8040216
1,3-Propanediol	RE - Puro	5l	P8040222
1,3-Propanediol	RE - Puro	190l	P8040268

Shuttle service

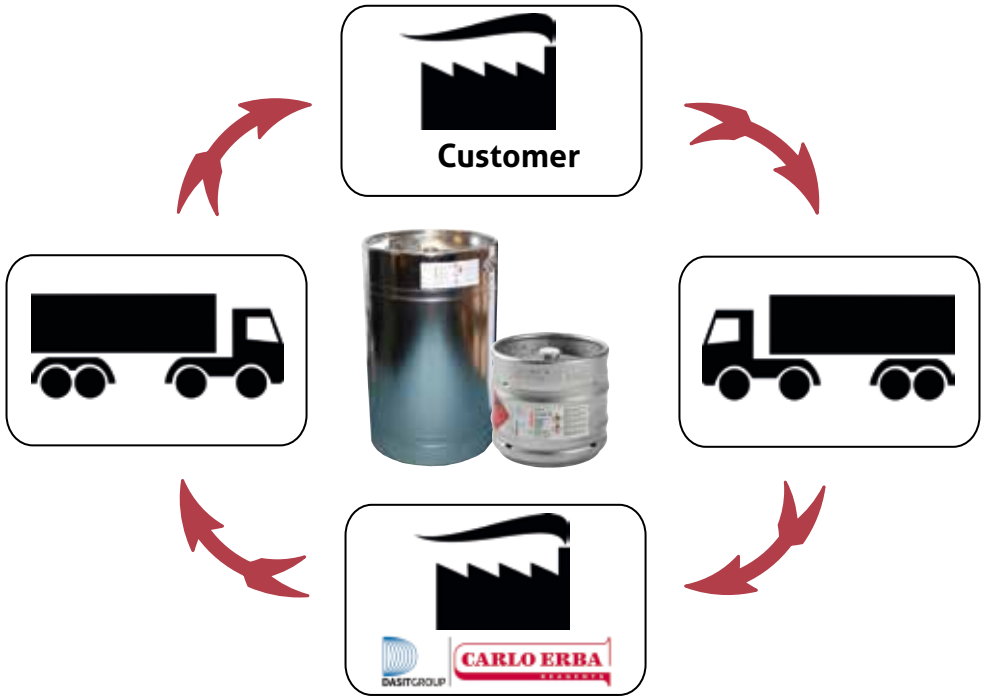
Stainless steel returnable containers to optimize solvent quality and the management of packaging waste

Improved safety

Easier handling and sampling thanks to a wide choice of connections.
Improved safety for the operators as well as for the process by reducing the exposure to solvents, o contaminated package waste to dispose of.

Environmental impact

Zero packaging waste, reduced environmental footprint.
Economy on the regulated destruction of disposable containers.



Quality preserved

The chemical compatibility in stainless steel shuttles is same as in glass and better than metal or plastic. Our stainless steel shuttle drums are fully welded, without crimping, a potential source of solvent contamination. All solvents are compatible with stainless steel, even for the highest qualities.

Efficient logistic

Each packaging is assigned to a single product and a single customer to reduce the risk of cross contamination. A defined number of shuttle drums is assigned to you based on your needs with regular rotations between your plant and ours. It is calculated on the amount of product required for your usage, the number of workstations, the duration of storage and the rotation frequency.

Shuttle packaging are available from 5 to 1000l. CARLO ERBA Reagents also offers a set of standard accessories and withdrawal systems including "on request" distribution or continuous push with nitrogen.

Download our dedicated brochure "Shuttle service" on our website

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