



# Methyltetrahydrofuran

## *A Good Replacement Solvent for Dichloromethane*

### Solvent Advantages

Dichloromethane (DCM) is a common solvent used for the production of many pharmaceutical and agricultural products. DCM like dichloroethane and other halogenated solvents is a highly regulated chemical. The use of DCM has been dropping primarily due to the NTP listing of DCM as a probable carcinogen<sup>1</sup> and its listing on California's Prop 65 as a known carcinogen. Also because DCM is very volatile, high losses to the atmosphere are common. 2-Methyltetrahydrofuran (MeTHF) is a versatile solvent that can be directly substituted for many of the production processes that require a polar solvent like DCM or dichloroethane.

MeTHF is produced from furfural which is a chemical derived from renewable sources (corn cobs, sugar cane bagasse, oat hulls). MeTHF has a number of properties that make it a good substitute for DCM.

- Limited miscibility with water facilitates easy product recovery
- Strong solvent for polar compounds typically soluble in DCM
- Very stable to basic conditions and stable to most acidic conditions
- In water systems, very clean phase separations are typically found
- Water washes decant from the reactor bottom versus DCM where water is the top layer
- Products in MeTHF can be dried in the reactor due to the favorable MeTHF azeotrope
- The 80 °C b.p. allows condensing with cooling water with little vapor loss

Some of the advantages of substituting MeTHF for DCM listed above are accompanied by higher than expected

reactivity in biphasic reactions. The higher apparent polarity in biphasic reactions is attributed to the dissolved water in the MeTHF phase.<sup>2</sup>

Products isolated in MeTHF can be conveniently dried because of the favorable MeTHF-water azeotrope. This can be done in a batch operation by refluxing the MeTHF phase of the condensed azeotrope. This procedure can also be used to dry MeTHF for recycle. Contact Penn for details on recycling MeTHF.

### Environmental, Health and Safety

MeTHF is a flammable liquid with a mildly irritating odor. MeTHF vapors, when mixed with air, are flammable when exposed to ignition sources. It should be handled only after consulting the material safety data sheet.

If spilled, MeTHF has a CERCLA reportable quantity of 100 pounds because of its low flash point. MeTHF could carry an EPA waste code of D001 for ignitability.

### Availability

MeTHF is available in bulk tank trucks, in 55 gallon steel drums (375 lbs; 170 kg) and 5 gallon steel pails (35 lbs, 16 kg).

### Shipping

The DOT HM 181 shipping name for MeTHF is methyltetrahydrofuran. It is a hazard class three (3) flammable liquid, Packing Group II material that requires a red flammable liquid label. The ID Number is UN 2536. Consult the MSDS for additional shipping information.

(1) <http://ehp.niehs.nih.gov/roc/tenth/profiles/s066dich.pdf>

(2) David H. Brown Ripin, Synlett 2003, No. 15, p2353.

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### Comparison of Properties of MeTHF and DCM

Property	MeTHF	DCM
Boiling point(°C).....	80.....	39.8
Freezing point (°C) .....	-136.....	-96.7
Density at 20 °C .....	0.855 .....	1.32
Viscosity at 25 °C (cps) .....	0.60 .....	0.43
Evaporation rate( <i>n</i> -butylacetate=1).....	4.2.....	27.5
Dielectric constant.....	7.0.....	10.7
Hildebrand solubility parameter .....	8.52 .....	9.95
Hansen Solubility Parameter		
Non-polar .....	8.3 .....	8.9
Polar.....	1.9 .....	3.1
Hydrogen bond .....	3.0.....	3.0
Total .....	8.9 .....	9.9
Solubility at 20 °C (wt %)		
In water .....	14 .....	1.32
Water in solvent .....	4.4 .....	0.14
Esters, alcohols, ketones, hydrocarbons, aromatics, chlorinated hydrocarbons.....	inf.....	inf
Flash point, TC(°C).....	-11.1 .....	none
Autoignition temperature (°C) .....	270.....	640
Water azeotrope		
boiling point (°C).....	71 .....	38.1
composition, wt% solvent .....	89.4.....	98.5
wt% water .....	10.6 .....	1.5

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