

# DMSO2

## Dimethyl Sulfone (DMSO2) Physical Properties

Bulletin # 301B

Octr 2007

### Introduction

Dimethyl sulfone has several common names: DMSO2, MSM, methylsulfonylmethane and methyl sulfone.

Dimethyl sulfone (DMSO2) has some unusual properties for an organic compound. It is a highly polar, high boiling, aprotic solvent that is a white crystalline solid at room temperature. DMSO2 will remain stable at high temperatures for extended amounts of time. Molten dimethyl sulfone is a solvent for a wide variety of compounds including organics, polymers and inorganic salts. A listing of available solubility information is included in this bulletin. The high solubility of many compounds in dimethyl sulfone as well as its high temperature stability makes it an ideal reaction solvent for reactions run best at high temperatures, with solvent properties similar to those of sulfolane. Removal is easily accomplished by sublimation.

Additionally, DMSO2 is not appreciably hygroscopic, and is extremely non-toxic.

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*Gaylord Chemical's solutions-based approach has contributed to the development and growth of industries including pharmaceuticals, hydrocarbons, electronics, polymers, coatings, agricultural chemicals, and industrial cleaners.*

*Gaylord Chemical's headquarters are located in Slidell, Louisiana with manufacturing, research, and development facilities in nearby Bogalusa, Louisiana. GCC remains the only producer of DMSO in the Western Hemisphere.*

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## **TYPICAL PHYSICAL PROPERTIES**

### **Dimethyl Sulfone, Methylsulfonylmethane\*, Methyl Sulfone**

Boiling point (at 760 mm Hg )	248°C (478°F)
Conductivity	0.47X10 <sup>-4</sup> ohm <sup>-1</sup> cm <sup>-1</sup>
Density, D110/4	1.1702 gm/cc
Dielectric constant (110°C)	47.39 MHZ
Dipole moment (20°C)	4.25 Debye
Flash point (Cleveland Open Cup)	143°C (290°F)
Hansen Solubility Parameters	
Polar	9.5
Hydrogen bonding	6.0
Non-polar	9.3
Heat of combustion (25°C) constant volume	-429.42 kcal/mole
Heat of formation (180°C)	-107.5 kcal/mole
Heat of fusion (9°C)	4.374 kcal/mole
Heat of sublimation (25°C, at 760 mm Hg )	18.4 kcal/mole
Heat of vaporization (25°C)	15.1 kcal/mole
Index of refraction (20°C)	1.4226
Melting Point at 760 mm Hg	109°C (228°F)
Molecular weight	94.13
Physical state	white, crystalline solid
Solubility parameter	14.5
Specific gravity (26°C)	1.450— 1.455
Specific heat (121°C) liquid	0.53 cal/gm/°C
Specific heat (25°C) solid	0.31 cal/gm/°C
Surface Tension	60.15 dynes/cm
Vapor pressure	
(112°C)	8.6 mm Hg
(250°C)	769.4 mm Hg
Viscosity, (125°C )	1.140 cP

\*International Union of Chemistry

## Solvent Characteristics of Dimethyl Sulfone Above the Melting Point of 109°C

### Acids

Acetic	sol.
Adipic	sol.
Anisic	sol.
Benzoic	sol.
Caprylic	sl. sol.
Fumaric	mod. sol.
Malonic	sol.
Succinic	sol.
Terephthalic	sl. sol.

### Alcohols and Glycols

Butyl alcohol	sol.
Cyclohexanol	sol.
Ethylene glycol	sol.
Ethylene Glycol monomethyl ether	sol.
Glycerol	sol.
1,5-Pentanediol sot	sol.
Propylene glycol sot	sol.
Triethylene glycol sot	sol.

### Amines

Aniline	sol.
Benzylamine	sol.
Carbazole	sol.
Dicyclohexylamine	sl. sol.
N, N-Dimethylaniline	sol.
Diphenylamine	sol.
Hexamethylenetetramine	decomposes
Propylenediamine	sol.
Pyridine	sol.
Tetraethylenepentamine	sol.
Triethylamine	sol.
Triethylenetetramine	sol.

### Anhydrides

Benzoic	sol.
Phthalic	sol.
Succinic	sol.

### Esters

Amyl acetate	sol.
Benzyl salicylate	sol.
Benzyl succinate	sol.
Butyl hexanoate	sol.
Methyl hexanoate	sol.
Methyl stearate	v. sl. sol.
Monacetin	sol.
Triacetin	sol.

### Ethers

Amyl	sol.
Ethylene glycol dimethyl ether	sol.

### Halogenated Compounds

Pentachlorobenzene	sl. sol.
Pentachlorophenol	sol.
1,1,2,2,-Tetrabromoethane	sol.
1,2,4-Trichlorobenzene	sol.
Trichlorocumene	sol.

### Hydrocarbons

Biphenyl	sol.
Mineral oil	insol.
Naphthalene	sol.

### Ketones

Anthraquinone	sol.
Benzil	sol.
Benzophenone	sol.
Diisobutylketone	sol.



### Solvent Characteristics of Dimethyl Sulfone Above the Melting Point of 109°C

#### Phenols

Catechol	sol.	Potassium bromide	sl. sol.
Naphthol	sol.	Potassium chloride	insol.
Phenol	sol.	Potassium ferricyanide	insol.
o-Phenylphenol	sol.	Potassium iodide	sol.
Phloroglucinol	sol.	Sodium acetate	v. sl. sol.
Pyrogallol	sol.	Sodium bromide	sl. sol.
Resorcinol	sol.	Sodium iodide	sol.

#### Salts

Ammonium chloride	v. sl. sol.	Sodium stearate	insol.
Calcium chloride	insol.	Uranyl nitrate	v. sol.

#### Other Compounds

Chromous chloride	sol.	Acetamide	sol.
Cobaltous acetate	sl. sol.	Benzaldehyde	sol.
Cobaltous chloride sot.	sol.	Butyraldehyde	sol.
Copper sulfate	insol.	3,4-Dimethoxyphenylacetonitrile	sol.
Ferric chloride	sol.	Nitrobenzene	sol.
Manganous chloride	v. sol.	p-Phenylnitrobenzene	sol.
Nickelous chloride	decomposes	Propionamide	sol.

### Solvent Characteristics of Dimethyl Sulfone Above the Melting Point of 109°C

#### Resins and Polymers

Amrez 1410 (phenol-formaldehyde)	insol.
Bakelite (phenol-formaldehyde)	insol.
Polybutylmethacrylate	insol.
Epon Resin #1007	sol.
Expandable polystyrene	insol.
GRS Rubber	insol.
Polyisobutylmethacrylate	sl. sol.
Melamine	sl.sol.
Melamine-formaldehyde (Parez 607)	insol.
Polymethylmethacrylate (Plexiglas)	sol.
Mylar	softens, insol.
Nylon	insol.

## **Solvent Characteristics of Dimethyl Sulfone Above the Melting Point of 109°C**

### **Resins and Polymers**

Paraffin	insoluble
Piccopale 70	slightly soluble
Polyacrylamide 50	insoluble
Polyacrylamide 100	insoluble
Polyacrylonitrile	soluble
Polyamide Resin #94	slightly soluble
Polybutylene 64	insoluble
Polyethylene, partially oxidized	slightly soluble
Polyvinyl alcohol 51-05	very slightly soluble
Polyvinyl butyral resin (Vinylite XYHL)	decomposes
Polyvinylidene chloride (Saran)	softens, insoluble
Polyvinylpyrrolidone	decomposes
Rosin	soluble
Rosin amine D	slightly soluble
Rosin amine D acetate	slightly soluble
Urea-formaldehyde (Uformite)	insoluble

### **Solubility of Dimethyl Sulfone in Organic Solvents Solvent**

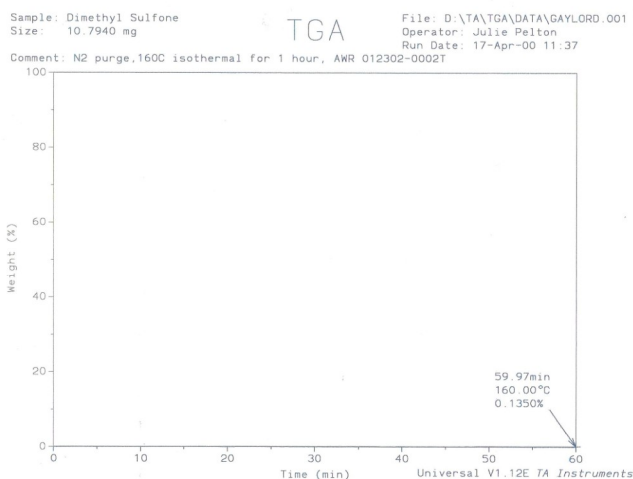
<u>Solvent</u>	<u>g/100 ml of Solvent</u>	<u>Solvent</u>	<u>g/100 ml Solvent</u>
Acetic acid, glacial	21.2 @25°C	Dioxane	12.4 @25°C
Acetone	15.36 @25°C	Ethyl alcohol	insol. @25°C, v. sol. @ 65-70°C
Benzene	2.2 @25°C, 6.6 @75°C	Formaldehyde, 37%	32.4 @25°C
Butyl cellusolve	12.2 @25°C	Isopropyl alcohol	1.03 @25°C, 4.52 @ 55°C
Carbon tetrachloride	insol. @25°C	Methyl alcohol	7.78 @25°C, 67.6 @ 60°C
Chloroform	9.4 @25°C	Methyl ethyl ketone	10.0 @25°C, 22.8 @65°C
Cyclohexane	trace @25°C, 4.7 @75°C	Methyl isobutyl ketone	1.93 @25°C, 8.8 @ 60°C
Diethyl ether	trace @25°C	2-Nitropropane	7.62 @25°C, 43.6 @ 70°C
Diethylene glycol	insol. @25°C, v. sol. @76°C	Petroleum ether	insol. @25°C
Dimethyl formamide	31.3 @25°C	Tetrahydrofuran	3.18 @25°C, 10.0 @52°C
Dimethyl sulfide	7.3 @25°C	Toluene	0.6 @25°C, 3.0 @ 92°C,
Dimethyl sulfoxide	48.5 @25°C	Xylene	0.36 @25°C, 2.4 @ 90°C



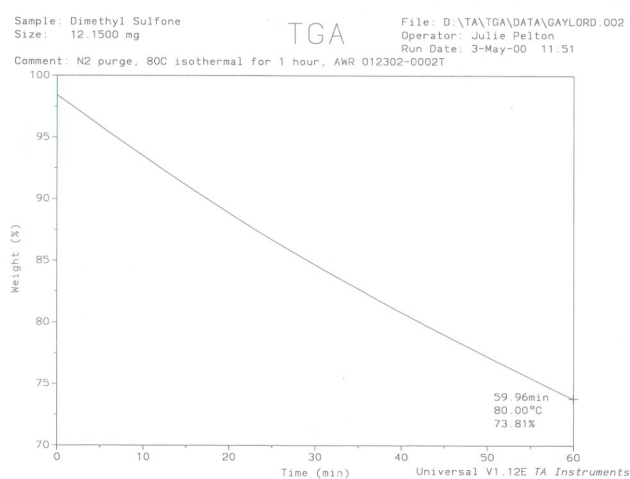
## Other Property Information

Dimethyl sulfone is a very stable compound. When heated in the presence of air at 140°C for 96 hours, purity as measured by gas chromatography (GC) revealed that less than 0.2 wt% of the sample had decomposed in this time. Heating dimethyl sulfone to 275 °C for one hour resulted in a decomposition of 0.03 mole percent. It did not decompose when heated to 238 °C for two hours in the presence of water and sodium hydroxide in an autoclave. Neither did it decompose when heated to 130 °C for three hours with a nitrating mixture of fuming sulfuric and fuming nitric acids. The proven stability of dimethyl sulfone at reflux temperature may well be its most valuable physical property. This suggests that dimethyl sulfone may be useful as a high temperature heat transfer fluid.

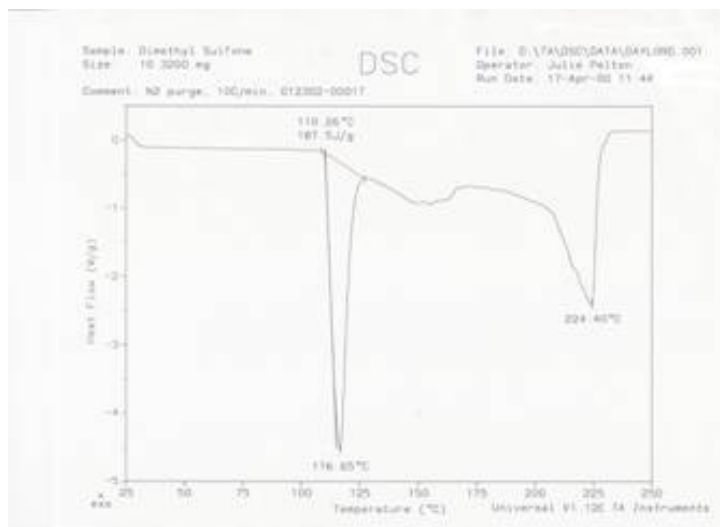
Regarding sublimation, Thermogravimetric Analysis (TGA) measurements suggest that DMSO<sub>2</sub> sublimates at the rate of 74 wt% / hour, at 80°C. At 160°C, all of the sample sublimated within a few minutes.



TGA analysis, beginning at 160C.



TGA analysis, beginning at 80C.



DSC analysis

DSC analysis detects the two phase changes of DMSO<sub>2</sub>, and suggests that vapor pressure of the molten sample is significant between the melting and boiling points of DMSO<sub>2</sub>.

To test hygroscopicity, a sample of DMSO<sub>2</sub> left in a humidity chamber set to 75% relative humidity gained only 0.1 % of its original weight after 30 days testing.

Dimethyl Sulfone can be used to extract aromatics from hydrocarbon mixtures. The addition of Dimethyl Sulfone to the solvents currently used in this process may enhance recovery and reduce the quantity of solvent required.

### TOXICITY OF DIMETHYL SULFONE

Limited toxicity studies and extensive observations give no signs of any toxicological problems. Dimethyl Sulfone is widely distributed in plants and animals and is the natural metabolic product from several sulfur-containing compounds. It has been isolated in beer, coffee, tea, *cladonia deformis* from peat bogs<sup>1</sup>, horse tail plant<sup>2</sup> human urine, cow's milk, dried cattle blood and adrenal glands .

The acute oral median lethal dose (LD<sub>50</sub>) of Dimethyl Sulfone was found to be > 17,020 mg/kg when administered as a 25.0% (w/v) aqueous solution to albino rats. In another study the LD of Dimethyl Sulfone given to mice by the oral route was >2,000 mg/kg. No deaths or clinical changes or body weight abnormalities were observed in this study<sup>4</sup>.

Dimethyl Sulfone when administered to New Zealand White rats by the dermal route, is to be considered "non-irritant" for the skin<sup>5</sup>. Also Dimethyl Sulfone administered to New Zealand White rats as a single ocular application, is to be considered "non irritant" for the eyes.<sup>6</sup>

The skin sensitization of Dimethyl Sulfone was assessed in guinea-pigs using the Magnusson test. No animals treated showed a positive reaction to the challenge<sup>7</sup>.

The mutagenic potential of Dimethyl Sulfone was investigated using the Ames Test. In the concentration range investigated, Dimethyl Sulfone did not show any mutagenic activity with or without the addition of S9 liver homogenate fractions<sup>8</sup>.

The toxicological and physiological properties of Dimethyl Sulfone have not been fully explored and reasonable care should be used in handling Dimethyl Sulfone.

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