# 

3-Methoxy-3-Methyl-1-Butanol



kuraray

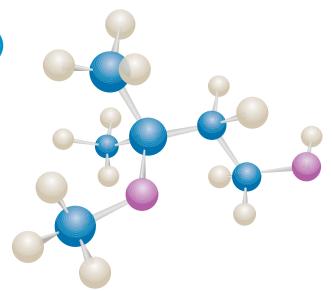


In 1972 KURARAY developed a new isoprene synthesis process by combining C4 and C1, this new process and another new synthetic rubber process provided KURARAY the incentive to build a new plant for these materials in Kashima.



# **MMB**

(3-Methoxy-3-Methyl-1-Butanol)



## Applications at a glance

- → Air Freshener
  Electrical, Fan, Car type, Reed diffuser, Gel, Aerosol...
- → Household Cleaner

  Kitchen, Air fan, Toilet, Bathroom, Floor, Multi purpose...
- → Industrial Cleaner

  for Electronic, PCB, Optical, Metal parts, Precision parts...

- → Dry Soap
- → Hand Cleaner
- → Insecticide and Pesticide
- → Ink and Coating





KURARAY'S KASHIMA FACILITY in Japan is under a strict quality control based on ISO-9001 and ISO-14001.

### The main reasons why using MMB

Low toxicity

Amphipathic

Good solubilizer

Mild odor

To control evaporation speed

Stable versus autoxidation

High Flash point

Biodegradable

Geringe Toxizität

Amphipatisch

Gutes Lösevermögen

Geruchsarm

Konstantes Verdampfungsverhalten

Stabil gegenüber Autoxidation

Hoher Flammpunkt

Biologisch abbaubar

Faible toxicité

**Amphiphile** 

Bonne propriété de solubilisation

Faible odeur

Permet un bon contrôle de la vitesse

d'évaporation

Stable à l'auto-oxydation

Point éclair élevé

Bonne biodégradabilité

Baja toxicidad

Anfipatico

Buena solubilidad

Bajo olor

Para controlar la velocidad de

evaporación

Estable frente a la oxidacion

Alto Punto de inflamación

Biodegradable

低毒性

両親媒性

溶解力

低臭気

安定した蒸発速度

耐酸化性

高引火点

生分解性

低毒

両親媒

溶解性好

低气味

穩定蒸発速率

耐酸化

高闪点

生物降解

### **Specification of MMB**

### **Appearance**

Clear and Colorless Liquid

### Color (APHA)

10 max

### Specific Gravity (20 °C / 20 °C)

0.925 - 0.930

### Distillation (760 mmHg)

IBP (°C) 168 min DP (°C) 178 max

### Acidity as acetic acid (Wt%)

0.01 max

### Water (%)

0.2 max





# **Properties of MMB**

### **Physical Properties**

Formula	$C_6H_{14}O_2 = 118$	
Specific Gravity (@ 20°C / 20°C)	0.927	
Specific Heat	2.30 J/g	0.549 cal/g
Viscosity (@ 20°C)	7.35 mPa•s	7.35 cps
Boiling Point (@ 760mmHg, 101 kPa)	174°C	345 °F
Heat of Vaporization (@ b.p.)	384 J/g	91.8 cal/g
Freezing Point	< -50°C	
Flash Point (Tag's CC)	68°C	154 ° F
Log Pow (@ 25°C)	0.18	
Solubility in Water	INFINITE	
Solubility Parameter	9.88 (cal/cm³)¹/²	
Hansen Solubility Parameter		
Dispersion	15.1 (MPa)¹/²	
Polar	4.7 (MPa) <sup>1/2</sup>	
Hydrogen Bonding	12.6 (MPa) <sup>1/2</sup>	
Total	20.2 (MPa) <sup>1/2</sup>	
Specific Electric Conductivity (@ 20°C)	8.6 x 10 <sup>-7</sup> Ω <sup>-1</sup> cm <sup>-1</sup>	
Vapor Density (air = 1)	4.1	
Refractive Index (@ 20°C)	1.4275	
Expansion Coefficient	0.00079/deg	
Surface Tension (@ 20°C)	29.9 mN/m	29.9 dyn/cm
Vapor Pressure (@ 20°C)	0.07 kPa	0.5 mmHg
Evaporation Rate (n-BuAc = 100)	7	
Explosion Range	1.2 - 13.1 vol %	
Ignition Point	395 °C	743 °F
Dilution Ratio		
a) Toluene (NC, 1/2 sec)	4.7	
b) Toluene (Epoxy resin)	4.5	
c) Xylene (NC, 1/2 sec)	4.3	

### **Effect on Plastics**

**Plastics** 

Rigid PVC	
Soft PVC	
Polyethylene (Low Density)	
Polyethylene (High Density)	
Polypropylene	
Polystyrene	
Polycarbonate	
Polyacetal	
PET	
PBT	
Polyphenylene Sulfide	

PET
PBT
Polyphenylene Sulfide
6-Nylon
6,6-Nylon
Teflon®
Epoxy Glass
Acrylic Resin
Phenol Resin
ABS

### Volume % vs Initial \* 8 9 0 0 0 19 0 0 0 0 0 0 0 0 0 Partially Dissolved 0 63

### **Effect on Elastomers**

### **Elastomers**

Fluoro Rubber Viton®
Chloroprene Rubber
Butyl Rubber
Nitrile Rubber
Silicone Rubber
Ethylene Propylene Rubber
Natural Rubber
Urethane Rubber
SBR

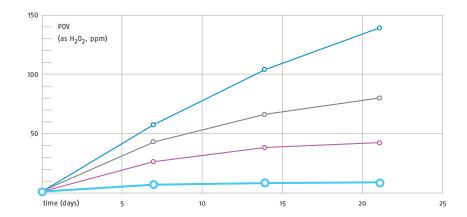
# Volume % vs Initial \* 82 64 0 115 6 7 17 129 26

<sup>\*</sup> Volume increase % of test specimen (50x20x2mm) after soaked in MMB at 50°C for 7 days.





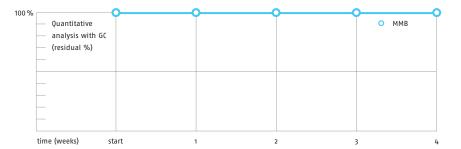
MMB is one of the fruits of our intensive development effort for novel products which are bio mimetic and at the same time friendlier to our environment and less harmful to living organisms.



### **Stability against Autoxidation**

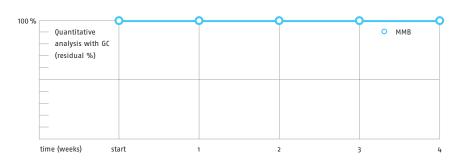
**Experimental:** Solvent (150 g) was placed in a beaker. Temperature was kept 18 °C to 22 °C. POV of each solvent was measured for 3 weeks by iodometric titration.

- O Ethylene oxide based Glycol ether -2
- O Ethylene oxide based Glycol ether -1
- O Propylene oxide based Glycol ether
- MMB



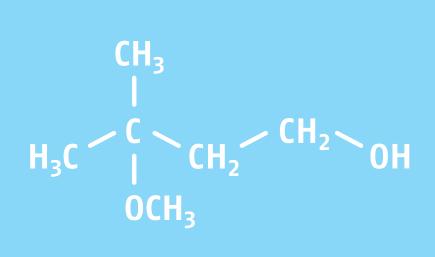
### Stability in Acidic Condition / pH = 4

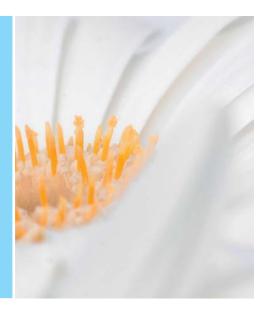
**Experimental:** MMB (50 g) and Phthalate buffer solution pH = 4.0 (50 g) were placed in a bottle and capped. The bottle was kept 50 °C for 4 weeks. Residual ratio was measured by GC analysis.



### Stability in Alkali Condition / pH = 10

**Experimental:** MMB (50 g) and Carbonate buffer solution pH = 10.0 (50 g) were placed in a bottle and capped. The bottle was kept 50 °C for 4 weeks. Residual ratio was measured by GC analysis.





### Safety Data of MMB

### 1. Acute Oral Toxicity

LD<sub>50</sub>: 4.30 g / kg (rats)<sup>1</sup> LD<sub>50</sub>: 5.83 g / kg (mice)<sup>2</sup>

### 2. Inhalation Toxicity after repeated dose<sup>2</sup>

(rats / 500 ppm / 28 days)

No significant changes were observed in the pathological, historical and functional examinations of viscera but a slight increase in GOT activity in liver and a slight increase in kidney weights as percentages of body weight. Other abdominal viscera showed nothing wrong in other examination.

Mutagenicity¹ (Reversion test with bacteria / Ames test)
 No evidence of mutagenic potential

### 4. Teratogenicity<sup>3</sup>

Developmental NOEL: 500 mg/kg - rat/day
Maternal NOEL: 250 mg/kg - rat/day
MMB is not a development toxicant, because there were
no adverse effects on development at either of two dosages
that were not toxic to the dams.

### 5. Acute Dermal Toxicity in Rats<sup>4</sup>

 $LD_{50}$ : > 2,000 mg / kg

No deaths occurred and no clinical signs were noted after  $24\,h$  dermal administration, under occlusion of MMB at a dose level of  $2,000\,mg\,l\,kg$ .

### 6. Skin sensitization potential4

Negative responses noted in all test and control group animals following challenge with MMB at concentration of 100 %.

### 7. Primary Skin Irritation in Rabbits<sup>4</sup>

MMB is non-irritant to rabbit skin under the test conditions. Mean irritation scores:

MMB 100 % : 0.04

MMB 50 % v/v in distilled water : 0.00

Very slight erythema was noted at one test site treated with MMB at a concentration of 100 % at the 24 h assessment only.

### 8. Dermal Irritation in Rabbits (28 day repeat)4

MMB 100 % : 0.6 (slightly irritant) MMB 50 % v/v in distilled water : 0.0

### 9. Photo-irritation potential in Guinea Pigs<sup>4</sup>

No photo-irritant responses were noted in the test and control groups.

### 10. Photosensitisation potential in Guinea Pigs 4

None of the test group animals showed a positive response.

### 11. Human Skin Patch Test<sup>5</sup>

48 h male & female: negative

### 12. Primary Eye Irritation in Rabbits<sup>5</sup>

MMB is moderately irritant to rabbit eyes, however, rising 30–60 s after instillation with distilled water reduces the irritation potential of MMB. The non-rinsed eyes showed some responses, and returned to normal by 9–10 days post instillation.

### References

- <sup>1</sup> Huntingdon Life Sciences, U.K.
- <sup>2</sup> Japan Industrial Safety Association, Japan
- <sup>3</sup> Argus Research Laboratory Inc., U.S.A.
- 4 Inveresk Research International, U.K.
- <sup>5</sup> Nihon Mouhatsu Kagaku Kyokai, Japan





MMB is a clear, colorless, low toxic water miscible liquid. In addition to MMB, Kuraray also produces, Diols, Diamine and Pesticide raw materials.

### **Environmental Effect of MMB**

1. Acute Toxicity for fish 1

(Killfish, 48 hrs JIS – K – 0102 – 55)

TLm: 7,400 ppm

2. Biomagnification in fish (carp, 8 weeks)

No magnification

3. Biodegradability<sup>2</sup>

MMB is biodegradable, in accordance with ISO 14593 (adopted March 1999), OECD 310 (adopted March 2006).

- → This test designed to meet the requirements of EC 648/2004 (amended by EC 907/2006), and EPA OPPTS 835.3120 (adopted January 1998)
- 4. Chemical Oxygen Demand (COD)<sup>3</sup>

8,060 mg/L (1% aqueous solution of MMB)

### References

- <sup>1</sup> Chemicals Inspection & Testing Institute, Japan
- <sup>2</sup> Huntingdon Life Sciences Ltd, U.K., 2008
- <sup>3</sup> Japan Oil Stuff Inspectors Corporation, Inc., Japan

### **Packaging**

16 kg (35 lbs) in can\* 185 kg (407 lbs) in drum 890 kg (1962 lbs) in IBC 19.9 MT in ISO container

\*available in Europe and Japan

### **Regulatory Status**

Methoxymethylbutanol

CAS Number	56539-66-3	
AICS (Australia) CRC-SEPA (China) DSL (Canada) ECL (Korea) EINECS (EU) ENCS (Japan) NZIOC (New Zealand) PICCS (Philippine) SWISS (Switzerland) TSCA (USA)	Listed Listed Listed Listed KE-24367 Listed 260-252-4 Listed 2-3079 Listed Listed Listed G-117002 Listed	
REACH	Pre-registered (Kuraray Europe GmbH has intention to register MMB in REACH as an importer)	
INCI Name:		



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