MMB

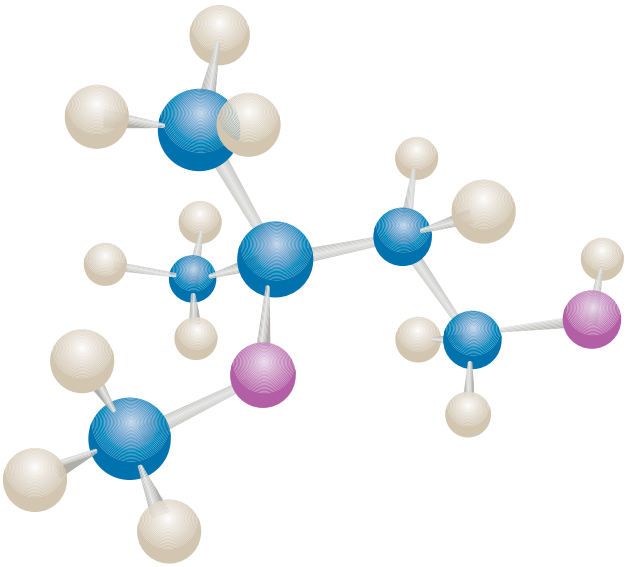
3-Methoxy-3-Methyl-1-Butanol

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	Geringe Toxizität
Amphipathic	Amphipatisch
Good solubilizer	Gutes Lösevermögen
Mild odor	Geruchsarm
To control evaporation speed	Konstantes Verdampfungsverhalten
Stable versus autoxidation	Stabil gegenüber Autoxidation
High Flash point	Hoher Flammpunkt
Biodegradable	Biologisch abbaubar

Faible toxicité	Baja toxicidad
Amphiphile	Anfipatico
Bonne propriété de solubilisation	Buena solubilidad
Faible odeur	Bajo olor
Permet un bon contrôle de la vitesse d'évaporation	Para controlar la velocidad de evaporación
Stable à l'auto-oxydation	Estable frente a la oxidacion
Point éclair élevé	Alto Punto de inflamación
Bonne biodégradabilité	Biodegradable

低毒性	低毒
両親媒性	両親媒
溶解力	溶解性好
低臭気	低气味
安定した蒸発速度	稳定蒸発速率
耐酸化性	耐酸化
高引火点	高闪点
生分解性	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 $(cal/cm^3)^{1/2}$	
Hansen Solubility Parameter		
Dispersion	15.1 $(MPa)^{1/2}$	
Polar	4.7 $(MPa)^{1/2}$	
Hydrogen Bonding	12.6 $(MPa)^{1/2}$	
Total	20.2 $(MPa)^{1/2}$	
Specific Electric Conductivity (@ 20 °C)	8.6 x $10^{-7}\Omega^{-1}cm^{-1}$	
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

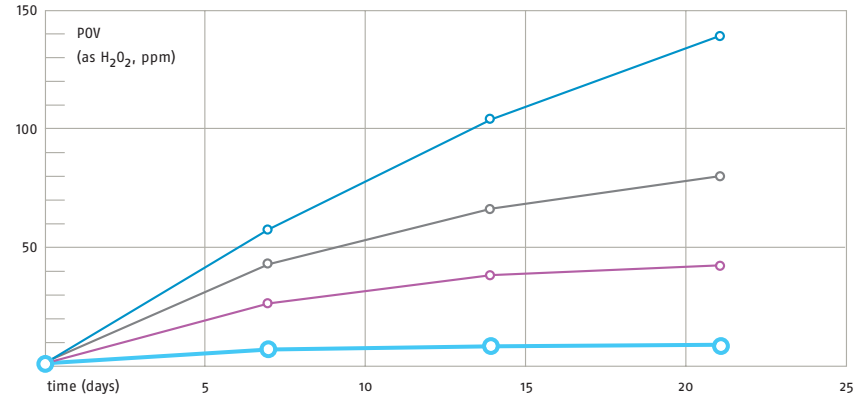
Plastics	Volume % vs Initial *
Rigid PVC	8
Soft PVC	9
Polyethylene (Low Density)	0
Polyethylene (High Density)	0
Polypropylene	0
Polystyrene	19
Polycarbonate	0
Polyacetal	0
PET	0
PBT	0
Polyphenylene Sulfide	0
6-Nylon	0
6,6-Nylon	0
Teflon®	0
Epoxy Glass	0
Acrylic Resin	Partially Dissolved
Phenol Resin	0
ABS	63

Effect on Elastomers

Elastomers	Volume % vs Initial *
Fluoro Rubber Viton®	82
Chloroprene Rubber	64
Butyl Rubber	0
Nitrile Rubber	115
Silicone Rubber	6
Ethylene Propylene Rubber	7
Natural Rubber	17
Urethane Rubber	129
SBR	26

* Volume increase % of test specimen (50 x 20 x 2 mm) after soaked in MMB at 50 °C for 7 days.

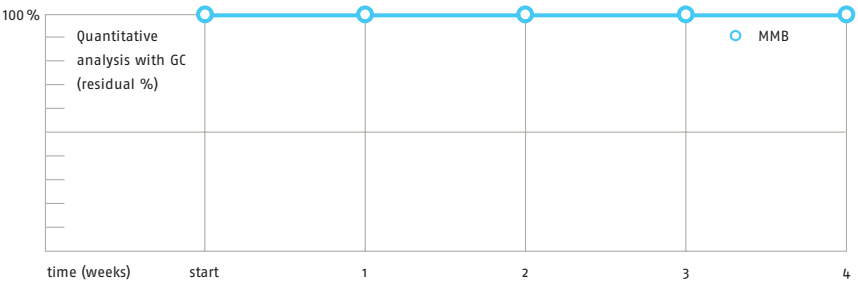
MMB is one of the fruits of our intensive development effort for novel products which are bio mimetic and at the same time friendlier to our environment and less harmful to living organisms.



Stability against Autoxidation

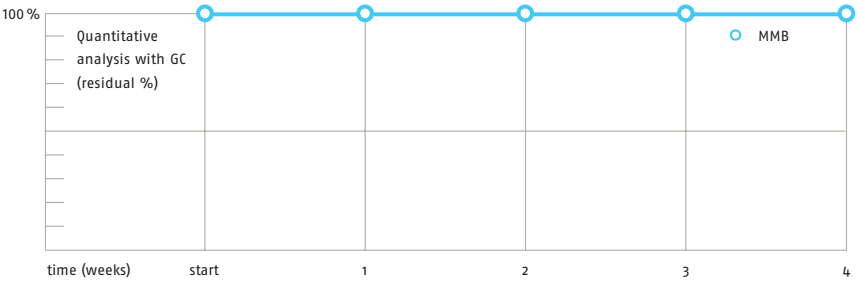
Experimental: Solvent (150 g) was placed in a beaker. Temperature was kept 18 °C to 22 °C. POV of each solvent was measured for 3 weeks by iodometric titration.

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



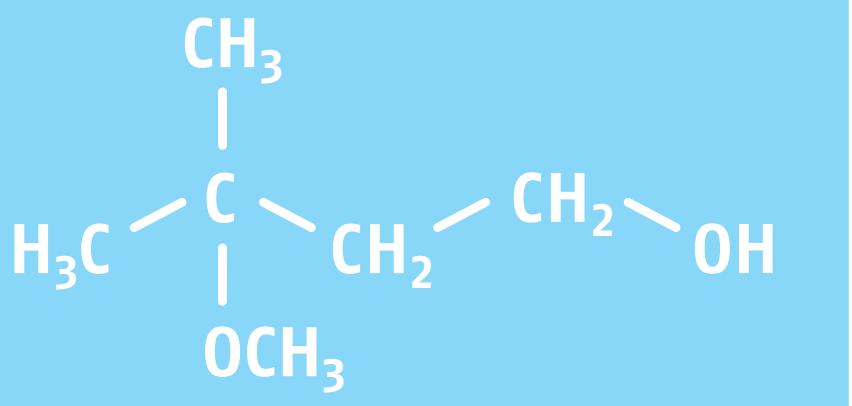
Stability in Acidic Condition / pH = 4

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_{50}: 4.30 g / kg (rats)[1]
   LD_{50}: 5.83 g / kg (mice)[2]

2. **Inhalation Toxicity after repeated dose**[2]
   (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.

3. **Mutagenicity**[1] (Reversion test with bacteria / Ames test)
   No evidence of mutagenic potential

4. **Teratogenicity**[3]
   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**[4]
   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 / kg .

6. **Skin sensitization potential**[4]
   Negative responses noted in all test and control group animals following challenge with MMB at concentration of 100 %.

7. **Primary Skin Irritation in Rabbits**[4]
   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**[4]
   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**[5]
    48 h male & female : negative

12. **Primary Eye Irritation in Rabbits**[5]
    MMB is moderately irritant to rabbit eyes, however, rinsing 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

[1] Huntingdon Life Sciences, U.K.
[2] Japan Industrial Safety Association, Japan
[3] Argus Research Laboratory Inc., U.S.A.
[4] Inveresk Research International, U.K.
[5] 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**[1] (carp, 8 weeks)
   No magnification

3. **Biodegradability**[2]
   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)**[3]
   8,060 mg / L (1 % aqueous solution of MMB)

References

[1] Chemicals Inspection & Testing Institute, Japan
[2] Huntingdon Life Sciences Ltd, U.K., 2008
[3] 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

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

INCI Name:
Methoxymethylbutanol

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