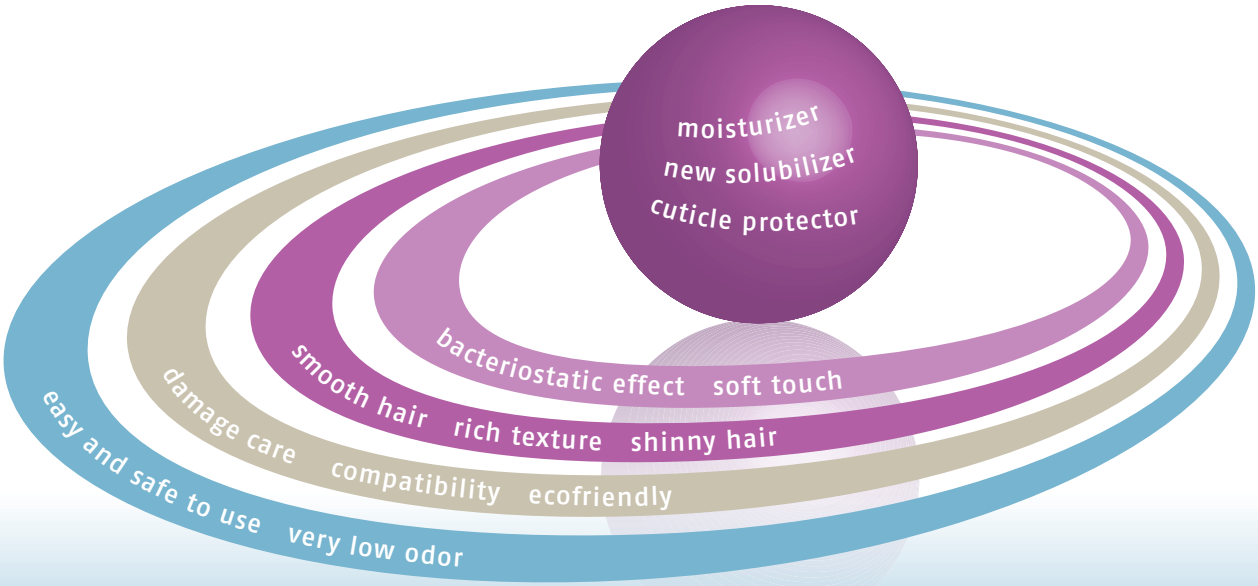
Isopentyldiol

3-Methyl-1,3-butanediol

kuraray

KURARAY has many unique isoprene and terpenoid derivatives with a high affinity to the human body. Indeed, not only Isopentyldiol, Citral and Synthetic Squalane are available but also custom-made pharmaceutical intermediates.

Isopentyldiol



Main applications

→ Hair Care

Hair conditioner,
Hair treatment,
Shampoo

→ Skin Care

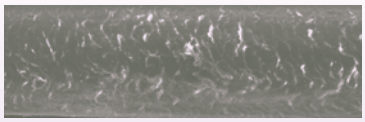
Skin milk, Moisture lotion,
Body soap, Make-up remover,
Eye & Lip care, Sunscreen

→ Decorative cosmetics

Eye shadow,
Moisturizing foundation,
Sunless tanning

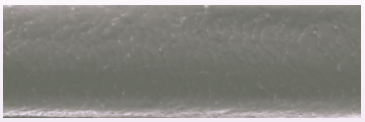
Technical Data – Effect on hair

Damaged hair / SEM x 430



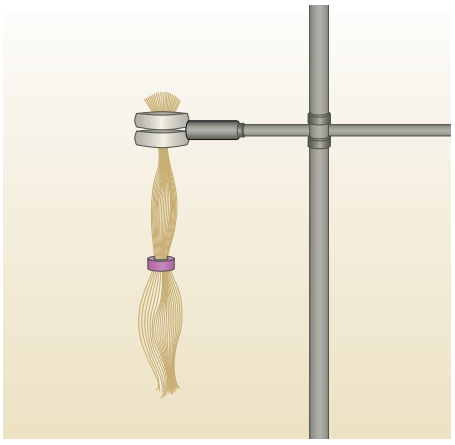
Rough cuticle due to damage

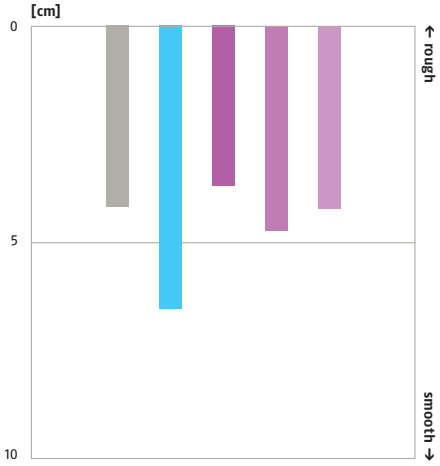
After treatment / SEM x 430



Damaged hair was treated with 5 % Isopentyldiol + 5 % Sorbitol for 30 minutes. Cuticle has become smooth again.

Tests done by Irfaq / France





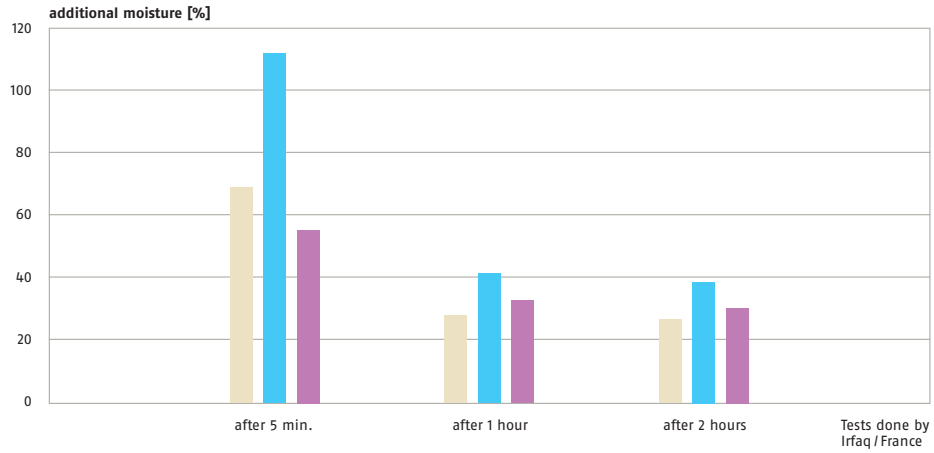
Tests done by Irfaq / France

Improve Smoothness of hair

The smoothness of hair is measured by a sliding ring test. Isopentyldiol shows a very good synergy with Sorbitol. A treatment with this mixture significantly improves sliding on damaged hair.

- Damaged and non treated hair
- with 5 % Isopentyldiol + 5 % Sorbitol
- with 5 % Propylene glycol + 5 % Sorbitol
- with 5 % Butylene glycol + 5 % Sorbitol
- with 2 % Hydrolyzed silk

Technical Data – Effect on skin



Moisturizer for skin: a long lasting effect

Skin moisture content is measured with a corneometer after treatment with skin creams containing either Isopentyldiol + Sorbitol, Sodium Hyaluronate, or no moisturizing agent. The combination with Isopentyldiol and Sorbitol maintains high skin moisture content.

- basic cream without moisturizing agent (control)
- basic cream with 5 % of Isopentyldiol + 5 % of Sorbitol
- basic cream with 0.5 % of Sodium Hyaluronate

	10 % Isopentyl-diol	10 % Propylene-glycol	10 % Hexylene-glycol	10 % Butylene-glycol	10 % Dipropy-leneglycol
Performance as makeup remover:					
Foundation	5	5	8	3	5
Lipstick	8	6	7	7	7
Skin freshness	7	5	6	6	5
Absence of stickiness	8	8	8	6	7
Appearance of the skin after makeup removal	8	8	8	8	8
Skin softness after makeup removal	8	8	8	7	7
Absence of tight feeling after makeup removal	8	8	8	8	8

Tests done by Irfaq / France

Make-up remover: Excellent performance, good feeling

A Make-up remover solution was prepared by diluting chemicals as a 10 % solution in water. Make-up remover pads were impregnated with 1 g of the solution to be tested and then applied 10 times to remove foundation and lipstick. A scoring was made by a panel of experts. Among these 5 chemicals, the solution made of 10 % Isopentyldiol showed an excellent performance at removing lipstick whilst maintaining a good skin condition after removing make-up.

○ 1 = poor ● 8 = good

According to Japanese standards, ISOPENTYLDIOL is regarded as a quasi-drug ingredient, thanks to its chemical safety.

Safety Data of Isopentyldiol

1. **Acute Toxicity – oral (1)**
   LD50 : > 5.00 g/kg (mice)
   (equivalent to OECD TG 401)

2. **Irritation – skin (1)**
   ➔ Non-irritating to Rabbits
   Primary Irritant Score : 0
   No irritant responses were noted following a 24 h exposure of Isopentyldiol. (variation of OECD TG 404, Compliant with US FDA Title 16, Section 1500.41)

3. **Irritation – eye (1)**
   ➔ Non-irritating to Rabbits
   No corneal, iridial or conjunctival responses were noted at any time during the test. (equivalent to OECD TG 405, Compliant with US FDA Title 16, Section 1500.42)

4. **Repeat dose Irritation (28 days) – skin (1)**
   ➔ Non-irritating to Rabbits
   In general, no skin irritation was noted.
   Very slight responses were noted on single occasions.
   No significant irritancy attributable to the test material was observed with histological evaluation.

5. **Skin sensitization (1)**
   (Magnusson-Kligman Maximisation test)
   ➔ Not sensitizing to Guinea pigs
   None of the test (Isopentyldiol: 50 %) or control group showed positive responses. (OECD TG 406)

6. **Photo irritation (1)**
   ➔ Non-irritating to Guinea pigs
   No photo-irritant responses were noted in the test (UV 320 – 400 nm, 20 J/cm²) and control groups.

7. **Photo sensitization (1)**
   ➔ Not sensitizing to Guinea pigs
   No positive effect was observed within 72 h after irradiation (UV-A, 10 J/cm²).

8. **Genotoxicity – bacterial reverse mutation test (1) (Ames test)**
   ➔ Non-mutagenic for *Salmonella typhimurium*, *Escherichia coli*
   No mutation was induced by 33 µg – 10,000 µg of Isopentyldiol / plate. (OECD TG 471)

9. **Genotoxicity – bacterial DNA repair assay (1)**
   (DNA repair test)
   ➔ Non-mutagenic for *Bacillus subtilis*
   No DNA damage repairable by *rec* gene products was induced by Isopentyldiol.

10. **Skin irritation – human volunteers (2)**
    ➔ Non-irritating to human
    No positive effect was observed for 30 participants within 48 h.

References:
(1) Inveresk Research International Ltd. / UK (1987)
(2) Japan Hair Science Association / Japan (1987)

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

Environmental Effect of Isopentyldiol

1. **Toxicity to fish (3)**
   LC50: > 103 mg/l (*Oncorhynchus mykiss* [rainbow trout],
   Exposure time: 96 h)
   (OECD Test Guideline 203)

2. **Toxicity to daphnia (3)**
   EC50: > 101 mg/l (Exposure time: 48 h)
   (OECD Test Guideline 202)

3. **Toxicity to aquaticplants (3)**
   IC50: > 95,8 mg/l (Growth inhibition)
   (OECD Test Guideline 201)

4. **Biodegradability (4)**
   ➔ Readily biodegradable.
   (OECD Test Guideline 301C)

5. **absorptive property to soil (3)**
   logKoc: < 1.3
   (OECD Test Guideline 121)

6. **Effect for activated sludge (3)**
   ➔ No effect (Activated Sludge, Respiration Inhibition Test)
   EC50(calculated): > 100 mg/L
   (OECD Test Guideline 209)

References:
(3) Huntingdon Life Science /UK
(4) Chemicals Inspection & Testing Institute, Japan (1993)

Packaging

195 kg (429 lbs) in drum
20 MT in ISO container

Regulatory Status

CAS Number	2568-33-4
CRC-SEPA (China)	Listed
ECL (Korea)	Listed KE-23542
ELINCS (EU)	Listed 459-270-7
REACH (EU)	Registered
ENCS (Japan)	Listed 2-240
NDSL (Canada)	Listed
PICCS (Philippine)	Listed
SWISS (Switzerland)	Listed 290800
TSCA (USA)	SNUR

INCI name: **Isopentyldiol**

Properties of Isopentyldiol

Physical Properties

Formula	$C_5H_{12}O_2$= 104	
Density (@ 20 °C)	0.979 g/cm³	
Viscosity (@ 20 °C)	250 mPa•s	
Dynamic viscosity (@ 20 °C)	~0.3 Pa•s	
Boiling Point (@ 760mmHg)	203 °C	397 °F
Freezing Point	< -50 °C	
Flash Point (COC)	116 °C	241 °F
Log Pow (@ 25 °C)	-0.56	
Solubility in Water	completely miscible	
Solubility Parameter	11.9 $(cal/cm^3)^{1/2}$	
Relative Vapor Density (air= 1)	3.6	
Refractive Index (@ 20 °C)	1.443	
Surface Tension (@ 20 °C, 1 g/L solution)	70 mN/m	70 dyn/cm
Vapor Pressure (@ 20 °C)	0.966 Pa	7.2 x 10^{-3} mmHg
Evaporation Rate (n-BuAc= 100)	< 1	
Explosion Range	0.8 - 24 vol %	
Ignition Point	> 400 °C	> 752 °F

Solubility of Isopentyldiol

Solute	solubitility
Water	> 100
Ethanol	> 100
Cetanol	> 100
Stearic acid	> 100
Olive oil	0.4
Glycerin monostearate	> 100
Glycerin tristearate	2
Cetyl ethylhexanoate	2.7
Trimethylstearylammonium chloride	> 100
POE(20) sorbitan mono stearate	> 100
Sodium POE lauryl ether sulfate	> 100
Sodium lauryl sulfate	> 100
Liquid paraffine	1.2
Squalane	0.8

Source: Kuraray Co., Ltd. (1987) **[wt % at 25 °C]**

Bacteriostatic properties

Concentration of Isopentyldiol [W/V %]	2.0	5.0	6.0	7.5	8.0	10.0	14.0	15.0	17.5	18.0	20.0	22.5	25.0
Escherichia coli		+		±		–		–					
Pseudomonas aeruginosa	+		±		±								
Staphylococcus aureus							+			±	–		
Candida albicans									±		±	±	–
Aspergillus niger									+		±	±	–

\+ Growth – No Growth

Source: Japan Food Research Laboratories

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Kuraray Co., Ltd.
Fine Chemicals Marketing and Sales Department
Tokyo Head office
Ote Center Building, 1-1-3, Otemachi
Chiyoda-ku, Tokyo, 100-8115 Japan
Phone + 81-3-67 01-16 21
Telefax + 81-3-67 01-16 46

Kuraray Europe GmbH
Building F 821, Höchst Industrial Park
65926 Frankfurt am Main, Germany
Phone + 49-69-30 53 58 44
+ 33-146-68 04 66
Telefax + 49-69-30 59 83 58 45

Kuraray America, Inc.
2625 Bay Area Boulevard, Suite 300
Houston, Texas 77058-1551 USA
Phone + 1-713-4 95 73 25
Telefax + 1-713-73 22

www.kuraray.co.jp/en/

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