

Opdyke, D.L.J., Food Cosmet. Toxicol., (suppl.), 1976, 14, 847, (methylene ether, レビユー, 性質)  
Higuchi, R. et al., Phytochemistry, 1977, 16, 1587, (Zingerone glucoside)  
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, VFP100

\*\*\*RTECS (化学物質毒性データ)\*\*\*

生体影響物質 :天然物. 一時刺激物質

\*\*\*健康障害に関するデータ\*\*\*

\*\*\*皮膚/眼の刺激に関するデータ\*\*\*

<<試験方法>> 標準ドライズ試験.

曝露経路 : 皮膚への塗布

被験動物 : げっ歯類-ウサギ.

投与量・期間: 500 mg/24 時間

反応の症度 : 中等度.

参照文献

FCTOD7 Food and Chemical Toxicology. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) V.20- 1982- [Vol.,頁,年(19-)]20,851,1982

\*\*\*急性毒性に関するデータ\*\*\*

<<試験方法>> LD50 試験 (50%致死量試験).

曝露経路 : 経口投与.

被験動物 : げっ歯類-ラット.

投与量・期間: 2580 mg/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参照文献

FCTOD7 Food and Chemical Toxicology. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) V.20- 1982- [Vol.,頁,年(19-)]20,851,1982

<<試験方法>> LD50 試験 (50%致死量試験).

曝露経路 : 皮膚への塗布

被験動物 : げっ歯類-ウサギ.

投与量・期間: >5 gm/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参照文献

FCTOD7 Food and Chemical Toxicology. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) V.20- 1982- [Vol.,頁,年(19-)]20,851,1982

\*\*\*米国に於ける状況\*\*\*

EPA TSCA Section 8(b) CHEMICAL INVENTORY

§ 2-[2-(3,4-Dihydroxyphenyl) ethyl] tetrahydro-6-(3,4,5-trihydroxyphenyl)-2H-pyran-4-ol; (2S,4R,6S)-form, 3',3''-Di-Me ether, 4-Ac

[CAS No.] 182227-92-5

[化合物分類] 単環芳香族 (Diarylalkyl), 含酸素複素環式化合物 (Pyran)

[構造式]

[分子式] C<sub>23</sub>H<sub>28</sub>O<sub>8</sub>

[分子量] 432.469

[正確な分子量] 432.17842

[基原] *Zingiber officinale*

[性状] オイル

[比旋光度]:  $[\alpha]_D^{25}$  -31.2 (c, 1.3 in EtOH)

[UV]: [neutral]  $\lambda_{max}$  226 (sh) (log  $\epsilon$  4.32); 280 (log  $\epsilon$  3.75) (EtOH)

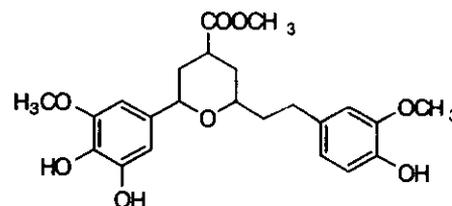
-----文献-----

Kikuzaki, H. et al., Phytochemistry, 1996, 43, 273, (分離, UV, IR, H-NMR, C13-NMR, Mas)

§ 2-[2-(3,4-Dihydroxyphenyl) ethyl] tetrahydro-6-(3,4,5-trihydroxyphenyl)-2H-pyran-4-ol; (2S,4R,6S)-form, 3',3'',5''-Tri-Me ether

[CAS No.] 182227-94-7

[化合物分類] 単環芳香族 (Diarylalkyl), 含酸素複素環式化合物 (Pyran)



[構造式]

[分子式] C<sub>22</sub>H<sub>26</sub>O<sub>7</sub>

[分子量] 404.459

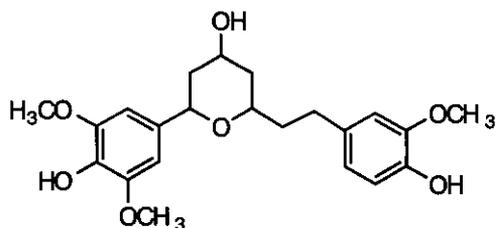
[正確な分子量] 404.183505

[基原] *Zingiber officinale*

[比旋光度]:  $[\alpha]_D^{25}$  -48.6 (c, 0.6 in EtOH)

[UV]: [neutral]  $\lambda_{max}$  226 (sh) (log  $\epsilon$  4.09); 280 (log  $\epsilon$

3.59) (EtOH)



-----文献-----

Kikuzaki, H. et al., *Phytochemistry*, 1996, 43, 273, (分離, UV, IR, H-NMR, C13-NMR, Mas)

§ 2-[2-(3,4-Dihydroxyphenyl)ethyl] tetrahydro-6-(3,4,5-trihydroxyphenyl)-2H-pyran-4-ol; (2S,4S,6S)-form, 3',3''-Di-Me ether

[CAS No.] 182369-54-6

[化合物分類] 単環芳香族 (Diarylalkyl), 含酸素複素環式化合物 (Pyran)

[構造式]

[分子式] C<sub>21</sub>H<sub>26</sub>O<sub>7</sub>

[分子量] 390.432

[正確な分子量] 390.167855

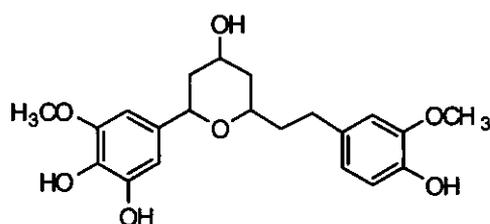
[基原] *Zingiber officinale*

[性状] オイル

[比旋光度]:  $[\alpha]_D^{25}$  -41.6 (c, 0.9 in EtOH)

[UV]: [neutral]  $\lambda_{max}$  225 (sh) (log  $\epsilon$  4.03); 280 (log  $\epsilon$

3.51) (EtOH)



-----文献-----

Kikuzaki, H. et al., *Phytochemistry*, 1996, 43, 273, (分離, UV, IR, H-NMR, C13-NMR, Mas)

§ 2-[2-(3,4-Dihydroxyphenyl)ethyl] tetrahydro-6-(3,4,5-trihydroxyphenyl)-2H-pyran-4-ol; (2S,4S,6S)-form, 3',3''-Di-Me ether, 4-Ac

[CAS No.] 182369-53-5

[化合物分類] 含酸素複素環式化合物 (Pyran), 単環芳香族 (Diarylalkyl)

[構造式]

[分子式] C<sub>23</sub>H<sub>28</sub>O<sub>8</sub>

[分子量] 432.469

[正確な分子量] 432.17842

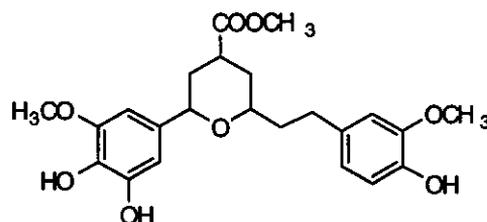
[基原] *Zingiber officinale*

[性状] オイル

[比旋光度]:  $[\alpha]_D^{25}$  -23.3 (c, 0.5 in EtOH)

[UV]: [neutral]  $\lambda_{max}$  226 (sh) (log  $\epsilon$  4.33); 280 (log  $\epsilon$

3.76) (EtOH)



-----文献-----

Kikuzaki, H. et al., *Phytochemistry*, 1996, 43, 273, (分離, UV, IR, H-NMR, C13-NMR, Mas)

§ 2,6-Dimethyl-2,6-octadiene-1,8-diol; (2E,6E)-form, 8-O-β-D-Glucopyranoside

[化合物分類] テルペノイド (Acyclic monoterpenoid)

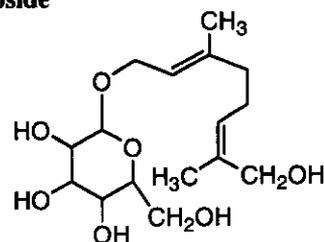
[構造式]

[分子式] C<sub>16</sub>H<sub>28</sub>O<sub>7</sub>

[分子量] 332.393

[正確な分子量] 332.183505

[基原] 新鮮なショウガ (*Zingiber officinale*)



-----文献-----

Bohlmann, F. et al., *Phytochemistry*, 1978, 17, 453, (bis-3-methylbutanoyl, di-Ac)

Jakupovic, J. et al., *Planta Med.*, 1991, 57, 450, (分離, H-NMR)

Abdel-Kader, M.S. et al., *Phytochemistry*, 1993, 34, 1367, (分離, H-NMR, C13-NMR)

Jaensch, M. et al., *Phytochemistry*, 1993, 34, 1367, (分離, H-NMR)  
Otsuka, H., *Phytochemistry*, 1994, 37, 461, (分離, H-NMR, C13-NMR)  
Sekiwa, Y. et al., *Biosci., Biotechnol., Biochem.*, 1999, 63, 384, (8-glucoside)

§ 2,6-Dimethyl-2,6-octadiene-1,8-diol; (2*E*,6*Z*)-form, 8-*O*-β-D-Glucopyranoside

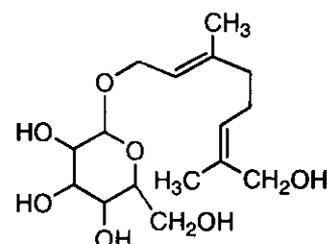
[化合物分類]テルペノイド (Acyclic monoterpeneoid)

[構造式]

[分子量] 332.393

[正確な分子量] 332.183505

[基原]新鮮なショウガ (*Zingiber officinale*)



-----文献-----

Bohlmann, F. et al., *Phytochemistry*, 1978, 17, 453, (bis-3-methylbutanoyl, di-Ac)  
Jakupovic, J. et al., *Planta Med.*, 1991, 57, 450, (分離, H-NMR)  
Abdel-Kader, M.S. et al., *Phytochemistry*, 1993, 34, 1367, (分離, H-NMR, C13-NMR)  
Jaensch, M. et al., *Phytochemistry*, 1993, 34, 1367, (分離, H-NMR)  
Otsuka, H., *Phytochemistry*, 1994, 37, 461, (分離, H-NMR, C13-NMR)  
Sekiwa, Y. et al., *Biosci., Biotechnol., Biochem.*, 1999, 63, 384, (8-glucoside)

§ 1,8-Epoxy-*p*-menthan-3-ol; (1*R*,3*S*,4*S*)-form, *O*-β-D-Glucopyranoside

[CAS No.] 155836-27-4

[化合物分類]テルペノイド (*p*-Menthane monoterpeneoid)

[構造式]

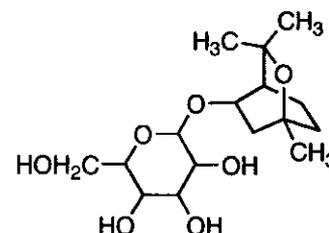
[分子式] C<sub>16</sub>H<sub>26</sub>O<sub>7</sub>

[分子量] 332.393

[正確な分子量] 332.183505

[基原]新鮮なショウガ (*Zingiber officinale*)

[比旋光度]: [α]<sub>D</sub><sup>23</sup> -21.7 (c, 0.52 in MeOH)



-----文献-----

Bondavalli, F. et al., *J.C.S. Perkin 1*, 1980, 2626, (合成法)  
de Boggianto, M.V. et al., *J.O.C.*, 1987, 52, 1505, (合成法)  
Asakawa, Y. et al., *Phytochemistry*, 1988, 27, 3861, (合成法, C13-NMR)  
Sekiwa, Y. et al., *Biosci., Biotechnol., Biochem.*, 1999, 63, 384, (分離, 配糖体)

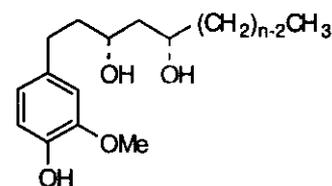
§ Gingerdiols

[化学名・別名] Gingediols

[関連 CAS No.] 39886-85-6, 99827-31-3

[構造式]

[基原]ショウガ (*Zingiber officinale*) の微量成分



-----文献-----

Murata, T. et al., *Chem. Pharm. Bull.*, 1972, 20, 2291, (分離, 構造決定, IR, H-NMR)  
Masada, Y. et al., *Yakugaku Zasshi*, 1974, 94, 735; *CA*, 81, 166345p, (分離)  
Kimura, I. et al., *Jpn. J. Pharmacol.*, 1988, 48, 257, (薬理)  
Kikuzaki, H. et al., *Phytochemistry*, 1992, 31, 1783, (分離, 構造決定)  
Juch, M. et al., *Helv. Chim. Acta*, 1997, 80, 436, (*Plectranthus acetate*)  
Sekiwa, Y. et al., *J. Agric. Food Chem.*, 2000, 48, 373, (6-Gingerdiol glucoside)

§ Gingerdiols; [6]-Gingerdiol, 5-*O*-β-D-Glucopyranoside

[化合物分類]脂肪族化合物 (Long-chain aromatic system)

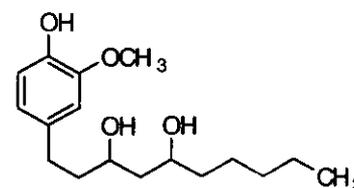
[構造式]

[分子式] C<sub>23</sub>H<sub>38</sub>O<sub>9</sub>

[分子量] 458.548

[正確な分子量] 458.251585

[基原] *Zingiber officinale*



[性状] オイル

[比旋光度]:  $[\alpha]_D^{24} -13.3$  (c, 0.72 in MeOH)

-----文献-----

Murata, T. et al., Chem. Pharm. Bull., 1972, 20, 2291, (分離, 構造決定, IR, H-NMR)

Masada, Y. et al., Yakugaku Zasshi, 1974, 94, 735; CA, 81, 166345p, (分離)

Kimura, I. et al., Jpn. J. Pharmacol., 1988, 48, 257, (薬理)

Kikuzaki, H. et al., Phytochemistry, 1992, 31, 1783, (分離, 構造決定)

Juch, M. et al., Helv. Chim. Acta, 1997, 80, 436, (Plectranthus acetate)

Sekiwa, Y. et al., J. Agric. Food Chem., 2000, 48, 373, (6-Gingerdiol glucoside)

§ Gingerdiols; [6]-Gingerdiol, 4'-O-β-D-Glucopyranoside

[化合物分類] 脂肪族化合物 (Long-chain aromatic system)

[構造式]

[分子式] C<sub>23</sub>H<sub>38</sub>O<sub>9</sub>

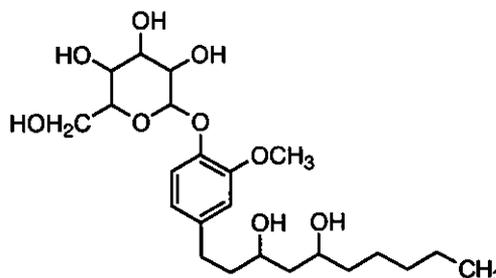
[分子量] 458.548

[正確な分子量] 458.251585

[基原] *Zingiber officinale*

[性状] 無定型の粉末

[比旋光度]:  $[\alpha]_D^{24} -29.3$  (c, 0.69 in MeOH)



-----文献-----

Murata, T. et al., Chem. Pharm. Bull., 1972, 20, 2291, (分離, 構造決定, IR, H-NMR)

Masada, Y. et al., Yakugaku Zasshi, 1974, 94, 735; CA, 81, 166345p, (分離)

Kimura, I. et al., Jpn. J. Pharmacol., 1988, 48, 257, (薬理)

Kikuzaki, H. et al., Phytochemistry, 1992, 31, 1783, (分離, 構造決定)

Juch, M. et al., Helv. Chim. Acta, 1997, 80, 436, (Plectranthus acetate)

Sekiwa, Y. et al., J. Agric. Food Chem., 2000, 48, 373, (6-Gingerdiol glucoside)

§ Gingerdiols; [6]-Gingerdiol, 3-Ac

[CAS No.] 143519-17-9

[化合物分類] 脂肪族化合物 (Long-chain aromatic system)

[構造式]

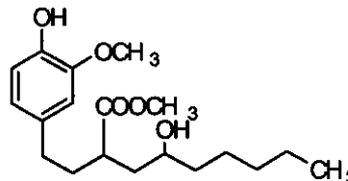
[分子式] C<sub>19</sub>H<sub>30</sub>O<sub>5</sub>

[分子量] 338.443

[正確な分子量] 338.209325

[基原] *Zingiber officinale*

[性状] オイル



-----文献-----

Murata, T. et al., Chem. Pharm. Bull., 1972, 20, 2291, (分離, 構造決定, IR, H-NMR)

Masada, Y. et al., Yakugaku Zasshi, 1974, 94, 735; CA, 81, 166345p, (分離)

Kimura, I. et al., Jpn. J. Pharmacol., 1988, 48, 257, (薬理)

Kikuzaki, H. et al., Phytochemistry, 1992, 31, 1783, (分離, 構造決定)

Juch, M. et al., Helv. Chim. Acta, 1997, 80, 436, (Plectranthus acetate)

Sekiwa, Y. et al., J. Agric. Food Chem., 2000, 48, 373, (6-Gingerdiol glucoside)

§ Gingerdiols; [6]-Gingerdiol, 5-Ac

[CAS No.] 143519-16-8

[化合物分類] 脂肪族化合物 (Long-chain aromatic system)

[構造式]

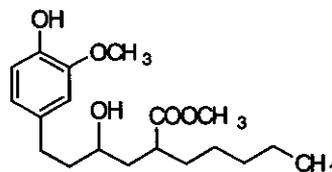
[分子式] C<sub>19</sub>H<sub>30</sub>O<sub>5</sub>

[分子量] 338.443

[正確な分子量] 338.209325

[基原] *Zingiber officinale*

[性状] オイル



-----文献-----

Murata, T. et al., Chem. Pharm. Bull., 1972, 20, 2291, (分離, 構造決定, IR, H-NMR)

Masada, Y. et al., Yakugaku Zasshi, 1974, 94, 735; CA, 81, 166345p, (分離)  
 Kimura, I. et al., Jpn. J. Pharmacol., 1988, 48, 257, (薬理)  
 Kikuzaki, H. et al., Phytochemistry, 1992, 31, 1783, (分離, 構造決定)  
 Juch, M. et al., Helv. Chim. Acta, 1997, 80, 436, (Plectranthus acetate)  
 Sekiwa, Y. et al., J. Agric. Food Chem., 2000, 48, 373, (6-Gingerdiol glucoside)

§ Gingerdiols; [6]-Gingerdiol, 3,5-Di-Ac

[CAS No.] 143615-75-2  
 [化合物分類] 脂肪族化合物 (Long-chain aromatic system)

[構造式]

[分子式]  $C_{21}H_{32}O_6$

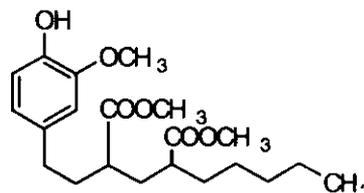
[分子量] 380.48

[正確な分子量] 380.21989

[基原] *Zingiber officinale*

[性状] オイル

[比旋光度]:  $[\alpha]_D^{20} -3.8$  (c, 0.5 in  $CHCl_3$ )



-----文献-----

Murata, T. et al., Chem. Pharm. Bull., 1972, 20, 2291, (分離, 構造決定, IR, H-NMR)  
 Masada, Y. et al., Yakugaku Zasshi, 1974, 94, 735; CA, 81, 166345p, (分離)  
 Kimura, I. et al., Jpn. J. Pharmacol., 1988, 48, 257, (薬理)  
 Kikuzaki, H. et al., Phytochemistry, 1992, 31, 1783, (分離, 構造決定)  
 Juch, M. et al., Helv. Chim. Acta, 1997, 80, 436, (Plectranthus acetate)  
 Sekiwa, Y. et al., J. Agric. Food Chem., 2000, 48, 373, (6-Gingerdiol glucoside)

§ Gingerdiols; [6]-Gingerdiol, 3'-Me ether, 3,5-di-Ac

[CAS No.] 143519-18-0  
 [化合物分類] 脂肪族化合物 (Long-chain aromatic system)

[構造式]

[分子式]  $C_{22}H_{34}O_6$

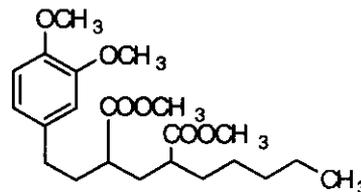
[分子量] 394.507

[正確な分子量] 394.23554

[基原] *Zingiber officinale*

[性状] オイル

[比旋光度]:  $[\alpha]_D^{24} -1.4$  (c, 0.7 in  $CHCl_3$ )

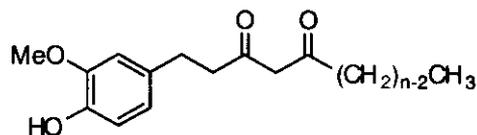


-----文献-----

Murata, T. et al., Chem. Pharm. Bull., 1972, 20, 2291, (分離, 構造決定, IR, H-NMR)  
 Masada, Y. et al., Yakugaku Zasshi, 1974, 94, 735; CA, 81, 166345p, (分離)  
 Kimura, I. et al., Jpn. J. Pharmacol., 1988, 48, 257, (薬理)  
 Kikuzaki, H. et al., Phytochemistry, 1992, 31, 1783, (分離, 構造決定)  
 Juch, M. et al., Helv. Chim. Acta, 1997, 80, 436, (Plectranthus acetate)  
 Sekiwa, Y. et al., J. Agric. Food Chem., 2000, 48, 373, (6-Gingerdiol glucoside)

§ Gingerdiones

[構造式]



[基原] ショウガ (*Zingiber officinale*) の同族化合物

-----文献-----

Denniff, P. et al., J.C.S. Perkin 1, 1981, 82, (合成法)  
 Harvey, D.J., J. Chromatogr., 1981, 212, 75  
 Kiuchi, F. et al., Chem. Pharm. Bull., 1982, 30, 754

§ Gingerdiones; [6]Gingerdione

[化学名・別名] 1-(4-Hydroxy-3-methoxyphenyl)-3,5-decanedione  
 [CAS No.] 61871-71-4

[化合物分類] 脂肪族化合物 (Long-chain aromatic system)

[構造式]

[分子式]  $C_{17}H_{24}O_4$

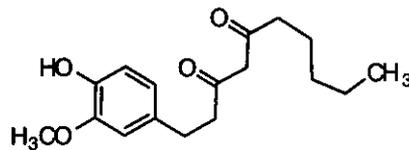
[分子量] 292.374

[正確な分子量] 292.16746

[基原] *Zingiber officinale*

[用途] プロスタグランジン抑制因子

[性状] オイル



-----文献-----

Denniff, P. et al., J.C.S. Perkin 1, 1981, 82, (合成法)

Harvey, D.J., J. Chromatogr., 1981, 212, 75

Kiuchi, F. et al., Chem. Pharm. Bull., 1982, 30, 754

### § Gingerdiones; [6]Gingerdione, 1',2'-Didehydro

[化学名・別名] [6]-Dehydrogingerdione

[CAS No.] 76060-35-0

[化合物分類] 脂肪族化合物 (Long-chain aromatic system)

[構造式]

[分子式]  $C_{17}H_{22}O_4$

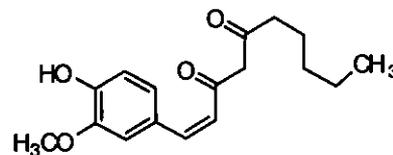
[分子量] 290.358

[正確な分子量] 290.15181

[基原] 次の植物から分離:*Zingiber officinale*

[性状] 黄色の針状結晶

[融点] Mp 83.5-84.5 °C



-----文献-----

Denniff, P. et al., J.C.S. Perkin 1, 1981, 82, (合成法)

Harvey, D.J., J. Chromatogr., 1981, 212, 75

Kiuchi, F. et al., Chem. Pharm. Bull., 1982, 30, 754

### § Gingerdiones; [8]Gingerdione

[化学名・別名] 1-(4-Hydroxy-3-methoxyphenyl)-3,5-dodecanedione (CAS 名)

[CAS No.] 77334-06-6

[化合物分類] 脂肪族化合物 (Long-chain aromatic system)

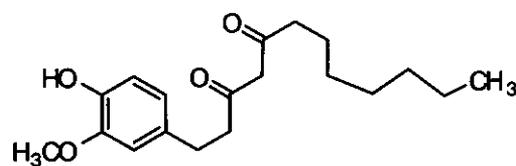
[構造式]

[分子式]  $C_{19}H_{28}O_4$

[分子量] 320.428

[正確な分子量] 320.19876

[基原] *Zingiber officinale*



-----文献-----

Denniff, P. et al., J.C.S. Perkin 1, 1981, 82, (合成法)

Harvey, D.J., J. Chromatogr., 1981, 212, 75

Kiuchi, F. et al., Chem. Pharm. Bull., 1982, 30, 754

### § Gingerdiones; [8]Gingerdione, 1,2-Didehydro

[化学名・別名] [8]-Dehydrogingerdione

[CAS No.] 77334-08-8

[化合物分類] 脂肪族化合物 (Long-chain aromatic system)

[構造式]

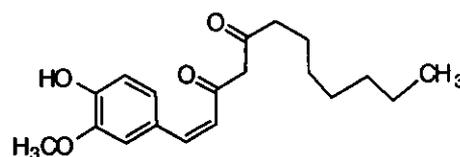
[分子式]  $C_{19}H_{26}O_4$

[分子量] 318.412

[正確な分子量] 318.18311

[基原] *Zingiber officinale*

[融点] Mp 48-49 °C



-----文献-----

Denniff, P. et al., J.C.S. Perkin 1, 1981, 82, (合成法)

Harvey, D.J., J. Chromatogr., 1981, 212, 75  
Kiuchi, F. et al., Chem. Pharm. Bull., 1982, 30, 754

§ Gingerdiones; [10] Gingerdione

[化学名・別名] 1-(4-Hydroxy-3-methoxyphenyl)-3,5-tetradecanedione

[化合物分類] 脂肪族化合物 (Long-chain aromatic system)

[構造式]

[分子式]  $C_{21}H_{32}O_4$

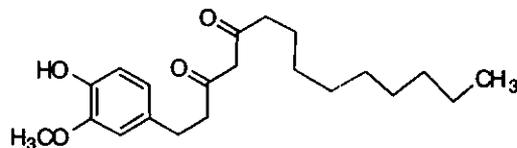
[分子量] 348.481

[正確な分子量] 348.23006

[基原] 次の植物から分離: *Zingiber officinale*

[用途] 強いプロスタグランジン抑制因子

[性状] 塊



-----文献-----

Denniff, P. et al., J.C.S. Perkin 1, 1981, 82, (合成法)

Harvey, D.J., J. Chromatogr., 1981, 212, 75

Kiuchi, F. et al., Chem. Pharm. Bull., 1982, 30, 754

§ Gingerdiones; [10] Gingerdione, 1',2'-Didehydro

[化学名・別名] [10]-Dehydrogingerdione

[CAS No.] 82206-04-0

[化合物分類] 脂肪族化合物 (Long-chain aromatic system)

[構造式]

[分子式]  $C_{21}H_{30}O_4$

[分子量] 346.466

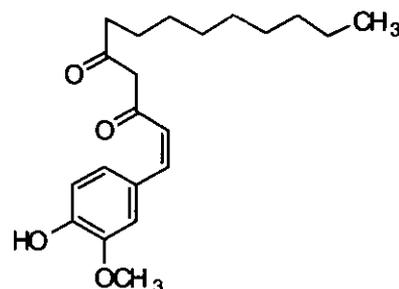
[正確な分子量] 346.21441

[基原] *Zingiber officinale*

[用途] プロスタグランジン抑制因子

[性状] 黄色の針状結晶

[融点] Mp 65-69.5 °C



-----文献-----

Denniff, P. et al., J.C.S. Perkin 1, 1981, 82, (合成法)

Harvey, D.J., J. Chromatogr., 1981, 212, 75

Kiuchi, F. et al., Chem. Pharm. Bull., 1982, 30, 754

§ Gingerdiones; [12] Gingerdione

[化学名・別名] 1-(4-Hydroxy-3-methoxyphenyl)

-3,5-hexadecanedione (CAS 名)

[CAS No.] 91815-31-5

[化合物分類] 脂肪族化合物 (Long-chain aromatic system)

[構造式]

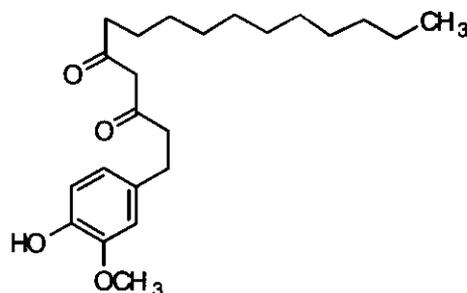
[分子式]  $C_{23}H_{36}O_4$

[分子量] 376.535

[正確な分子量] 376.26136

[基原] *Zingiber officinale*

[融点] Mp 44-45 °C



-----文献-----

Denniff, P. et al., J.C.S. Perkin 1, 1981, 82, (合成法)

Harvey, D.J., J. Chromatogr., 1981, 212, 75

Kiuchi, F. et al., Chem. Pharm. Bull., 1982, 30, 754

§ Gingerenone A

[化学名・別名] 1,7-Bis(4-hydroxy-3-methoxyphenyl)-4-hepten-3-one (CAS 名)

[CAS No.] 128700-97-0

[化合物分類] 単環芳香族 (Diarylalkyl)

[構造式]

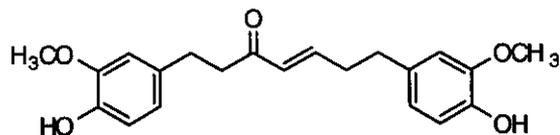
[分子式]  $C_{21}H_{24}O_5$

[分子量] 356.418

[正確な分子量] 356.162375

[基原] *Zingiber officinale*

[性状] オイル



-----文献-----

Terazawa, M. et al., Mokuzaï Gakkaishi, 1973, 19, 45; CA, 78, 84730j, (Hirsutenone)

Endo, K. et al., Phytochemistry, 1990, 29, 797, (分離, H-NMR, C13-NMR)

### § Gingerenone A; 5'-Methoxy

[化学名・別名] Isogingerenone B

[CAS No.] 128700-99-2

[化合物分類] 単環芳香族 (Diarylalkyl)

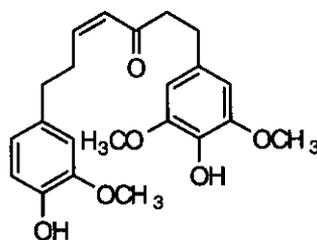
[構造式]

[分子式]  $C_{22}H_{26}O_6$

[分子量] 386.444

[正確な分子量] 386.17294

[基原] *Zingiber officinale*



-----文献-----

Terazawa, M. et al., Mokuzaï Gakkaishi, 1973, 19, 45; CA, 78, 84730j, (Hirsutenone)

Endo, K. et al., Phytochemistry, 1990, 29, 797, (分離, H-NMR, C13-NMR)

### § Gingerenone A; 5''-Methoxy

[化学名・別名] Gingerenone B

[CAS No.] 128700-98-1

[化合物分類] 単環芳香族 (Diarylalkyl)

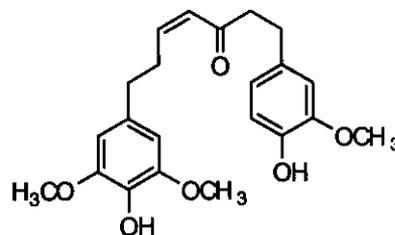
[構造式]

[分子式]  $C_{22}H_{26}O_6$

[分子量] 386.444

[正確な分子量] 386.17294

[基原] *Zingiber officinale*



-----文献-----

Terazawa, M. et al., Mokuzaï Gakkaishi, 1973, 19, 45; CA, 78, 84730j, (Hirsutenone)

Endo, K. et al., Phytochemistry, 1990, 29, 797, (分離, H-NMR, C13-NMR)

### § Gingerenone A; 3''-Demethoxy

[化学名・別名] Gingerenone C

[CAS No.] 128701-01-9

[化合物分類] 単環芳香族 (Diarylalkyl)

[構造式]

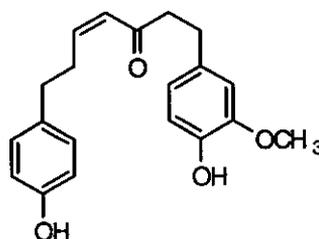
[分子式]  $C_{20}H_{22}O_4$

[分子量] 326.391

[正確な分子量] 326.15181

[基原] *Zingiber officinale*

[性状] オイル



-----文献-----

Terazawa, M. et al., Mokuzaï Gakkaishi, 1973, 19, 45; CA, 78, 84730j, (Hirsutenone)

Endo, K. et al., Phytochemistry, 1990, 29, 797, (分離, H-NMR, C13-NMR)

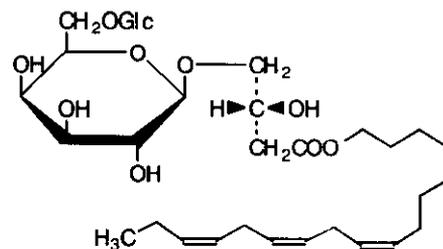
### § Gingerglycolipid A

[CAS No.] 145937-22-0

[化合物分類] 炭水化物 (Disaccharide), 脂肪族化合物 (Glycolipid)

[構造式]

[分子式]  $C_{33}H_{56}O_{14}$   
 [分子量] 676.797  
 [正確な分子量] 676.36701  
 [基原] *Zingiber officinale* (シヨウガ科)  
 [性状] 粉末  
 [比旋光度]:  $[\alpha]_D^{20} +37.7$  (c, 10 in MeOH)

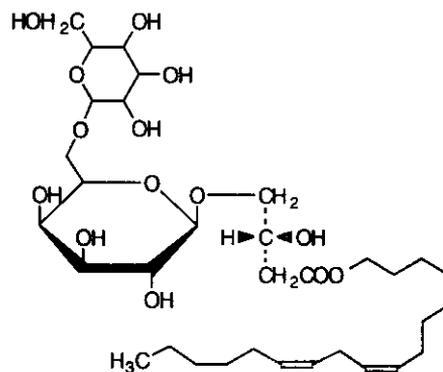


-----文献-----

Baruah, P. et al., *Phytochemistry*, 1983, 22, 1741, (分離, H-NMR)  
 Yoshikawa, M. et al., *Chem. Pharm. Bull.*, 1994, 42, 1226, (分離, H-NMR, C13-NMR)

### § Gingerglycolipid A; 15',16'-Dihydro

[化学名・別名] Gingerglycolipid B  
 [CAS No.] 88168-90-5  
 [化合物分類] 炭水化物 (Disaccharide), 脂肪族化合物 (Glycolipid)  
 [構造式]  
 [分子式]  $C_{33}H_{56}O_{14}$   
 [分子量] 678.813  
 [正確な分子量] 678.38266  
 [基原] *Zingiber officinale* (シヨウガ科), *Sonchus arvensis* (キク科)  
 [性状] 粉末  
 [比旋光度]:  $[\alpha]_D^{20} +50.9$  (c, 7.5 in MeOH)

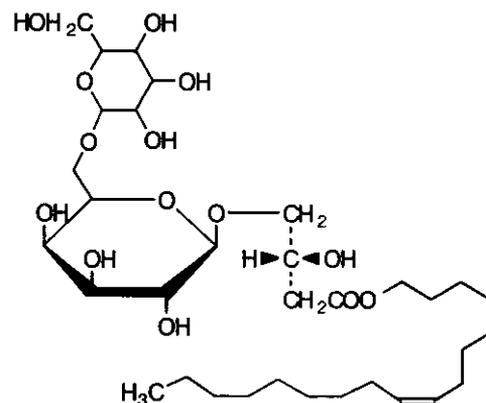


-----文献-----

Baruah, P. et al., *Phytochemistry*, 1983, 22, 1741, (分離, H-NMR)  
 Yoshikawa, M. et al., *Chem. Pharm. Bull.*, 1994, 42, 1226, (分離, H-NMR, C13-NMR)

### § Gingerglycolipid A; 12',13',15',16'-Tetrahydro

[化学名・別名] Gingerglycolipid C  
 [CAS No.] 35949-86-1  
 [化合物分類] 脂肪族化合物 (Glycolipid) 炭水化物 (Disaccharide)  
 [構造式]  
 [分子式]  $C_{33}H_{60}O_{14}$   
 [分子量] 680.829  
 [正確な分子量] 680.39831  
 [基原] *Zingiber officinale* (シヨウガ科)  
 [性状] 粉末  
 [比旋光度]:  $[\alpha]_D^{20} +26.9$  (c, 10 in MeOH)



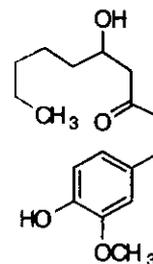
-----文献-----

Baruah, P. et al., *Phytochemistry*, 1983, 22, 1741, (分離, H-NMR)  
 Yoshikawa, M. et al., *Chem. Pharm. Bull.*, 1994, 42, 1226, (分離, H-NMR, C13-NMR)

### § [6]-Gingerol; (S)-form

[CAS No.] 23513-14-6  
 [化合物分類] 単環芳香族 (Simple phenol)  
 [構造式]

[基原] シヨウガ *Zingiber officinale*  
 [性状] 刺激性の黄色オイル  
 [比旋光度]:  $[\alpha]_D +26.5$  (c, 1 in  $CHCl_3$ )  
 [UV]: [neutral]  $\lambda_{max}$  282 ( $\epsilon$  2560) (MeOH) [neutral]  $\lambda_{max}$  211 ; 282 (EtOH)  
 [化学物質毒性データ総覧 (RTECS) 登録番号] HE0757000



-----文献-----

Connell, D.W. et al., Aust. J. Chem., 1969, 22, 1033, (分離, 構造決定)  
Enders, D. et al., Chem. Ber., 1979, 112, 3703, (合成法)  
Denniff, P. et al., J.C.S. Perkin 1, 1980, 2637, (生合成)  
Giovanni, B.P. et al., J.C.S. Perkin 1, 1982, 2983, (合成法)  
Kato, N. et al., Chem. Pharm. Bull., 1984, 32, 1679, (合成法)  
Solladie, G. et al., J.O.C., 1993, 58, 2181, (合成法, 成書)  
Fleming, S.A. et al., Synth. Commun., 1999, 29, 1933, (合成法, H-NMR, C13-NMR)

\*\*\*RTECS (化学物質毒性データ)\*\*\*

生体影響物質 : 変異原物質

\*\*\*健康障害に関するデータ\*\*\*

\*\*\*急性毒性に関するデータ\*\*\*

<<試験方法>> LD50 試験 (50%致死量試験).

曝露経路 : 経口投与.

被験動物 : げっ歯類-マウス

投与量・期間 : 250 mg/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参照文献

JOPHDQ Journal of Pharmacobio-Dynamics. (Japan Pub. Trading Co. (USA), 1255 Howard St., San Francisco, CA 94103) V.1- 1978- [Vol.,頁,年(19-)]7,836,1984

<<試験方法>> LD50 試験 (50%致死量試験).

曝露経路 : 腹腔内投与

被験動物 : げっ歯類-マウス

投与量・期間 : 58100 ug/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参照文献

JOPHDQ Journal of Pharmacobio-Dynamics. (Japan Pub. Trading Co. (USA), 1255 Howard St., San Francisco, CA 94103) V.1- 1978- [Vol.,頁,年(19-)]7,836,1984

<<試験方法>> LD50 試験 (50%致死量試験).

曝露経路 : 静脈注射

被験動物 : げっ歯類-マウス

投与量・期間 : 25500 ug/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参照文献

JOPHDQ Journal of Pharmacobio-Dynamics. (Japan Pub. Trading Co. (USA), 1255 Howard St., San Francisco, CA 94103) V.1- 1978- [Vol.,頁,年(19-)]7,836,1984

\*\*\*変異原性に関するデータ\*\*\*

<<試験方法>> 微生物を用いた突然変異試験.

試験系 : 大腸菌 Salmonella typhimurium.

投与量・期間 : 50 mg/L

参照文献

MUREAV Mutation Research. (Elsevier Science Pub. B.V., POB 211, 1000 AE Amsterdam, Netherland) V.1- 1964- [Vol.,頁,年(19-)]103,119,1982

<<試験方法>> 微生物を用いた突然変異試験.

試験系 : 大腸菌 Salmonella typhimurium.

投与量・期間 : 5 ug/plate

参照文献

CALEDQ Cancer Letters (Shannon, Ireland). (Elsevier Scientific Pub. Ireland Ltd., POB 85, Limerick, Ireland) V.1- 1975- [Vol.,頁,年(19-)]36,221,1987

<<試験方法>> 微生物を用いた突然変異試験.

試験系 : 大腸菌 Escherichia coli

投与量・期間 : 200 umol/L

参照文献

MUREAV Mutation Research. (Elsevier Science Pub. B.V., POB 211, 1000 AE Amsterdam, Netherland) V.1- 1964- [Vol.,頁,年(19-)]122,87,1983

### § [8]-Gingerol; (S)-form

[CAS No.] 23513-08-8

[化合物分類] 単環芳香族 (Simple phenol), 脂肪族化合物 (Saturated unbranched aldehydes and ketone)

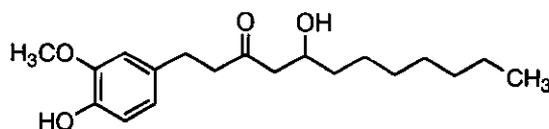
[構造式]

[基原] ショウガ, *Zingiber officinale* の根茎

[用途] 強心活性を示す

[融点] Mp 29-30 °C

[比旋光度]:  $[\alpha]_D^{25} +26$  (c, 0.9 in CHCl<sub>3</sub>)



-----文献-----

Cornell, D.W. et al., Aust. J. Chem., 1969, 22, 1033, (分離, 構造決定)

Shogi, N. et al., J. Pharm. Sci., 1982, 71, 1174, (分離, UV, H-NMR, C13-NMR)

Kato, N. et al., Chem. Pharm. Bull., 1984, 32, 1679, (合成法)

Martin, M. et al., Chirality, 1991, 3, 151, (enantiomers, 合成法, IR, H-NMR)

Solladie, G. et al., J.O.C., 1993, 58, 2181, (合成法, H-NMR, C13-NMR)

Fleming, S.A. et al., Synth. Commun., 1999, 29, 1933, (合成法, H-NMR, C13-NMR)

### § [10]-Gingerol; (S)-form

[CAS No.] 23513-15-7

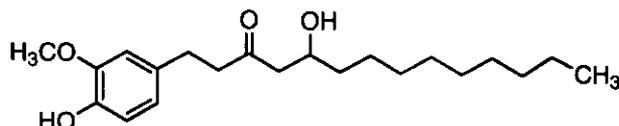
[化合物分類] 脂肪族化合物 (Saturated unbranched aldehydes and ketone), 単環芳香族 (Simple phenol)

[構造式]

[基原] ショウガ, *Zingiber officinale* の根茎

[融点] Mp 45-46 °C

[比旋光度]:  $[\alpha]_D^{25} +22.7$  (c, 1.02 in CHCl<sub>3</sub>)



-----文献-----

Cornell, D.W. et al., Aust. J. Chem., 1969, 22, 1033, (分離, 構造決定)

Shogi, N. et al., J. Pharm. Sci., 1982, 71, 1174, (分離, UV, H-NMR, C13-NMR)

Kato, N. et al., Chem. Pharm. Bull., 1984, 32, 1679, (合成法)

Solladie, G. et al., J.O.C., 1993, 58, 2181, (合成法, H-NMR, C13-NMR)

Fleming, S.A. et al., Synth. Commun., 1999, 29, 1933, (合成法, H-NMR, C13-NMR)

### § [12]-Gingerol

[化学名・別名] 5-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-hexadecanone (CAS 名)

[CAS No.] 104264-55-3

[その他の CAS No.] 77333-95-0, 107257-19-2

[構造式] As [6]-Gingerol with n = 10

[分子式] C<sub>23</sub>H<sub>38</sub>O<sub>4</sub>

[分子量] 378.551

[正確な分子量] 378.27701

[基原] *Zingiber officinale*. 次に示す物質の成分: Gan Jiang

-----文献-----

Kato, N. et al., Chem. Pharm. Bull., 1984, 32, 1679-1682, (合成法)

Chen, C.C. et al., J. Chromatogr., 1986, 360, 163-173, (分離)

### § 6-Gingesulfonic acid

[CAS No.] 145937-21-9

[化合物分類] 脂肪族化合物 (Long-chain aromatic system)

[構造式]

[分子式] C<sub>17</sub>H<sub>26</sub>O<sub>6</sub>

[分子量] 358.455

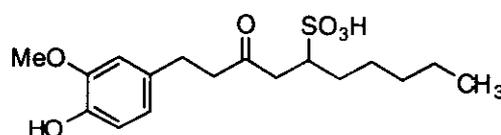
[正確な分子量] 358.14501

[基原] 次の植物の根茎から分離: *Zingiber officinale* (ショウガ)

[用途] 抗潰瘍薬

[性状] 粉末

[比旋光度]:  $[\alpha]_D^{25} -1$  (MeOH)



-----文献-----

Yoshikawa, M. et al., Chem. Pharm. Bull., 1994, 42, 1226

**§ 2-Heptanol (CAS 名)**

[化学名・別名] 1-Methylhexanol. FEMA 3288

[CAS No.] 543-49-7

[関連 CAS No.] 5921-82-4, 54638-12-9

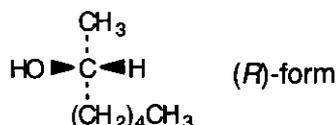
[化合物分類] 脂肪族化合物 (Saturated unbranched alcohol)

[構造式]

[分子式] C<sub>7</sub>H<sub>16</sub>O

[分子量] 116.203

[正確な分子量] 116.120115



[基原] *Zingiber officinale*, *Fragaria vesca*, *Catharanthus roseus* のオイルに存在する。 *Curvularia falcata* と *Mucor spp.* によって放出される

[傷害・毒性] 眼と皮膚を刺激する。 50 %致死量 (LD<sub>50</sub>) (ラット, 経口) 2580 mg/kg. 発火点: 71 °C

[化学物質毒性データ総覧 (RTECS) 登録番号] MJ2975000

-----文献-----

Aldrich Library of FT-IR Spectra, 1st edn., 1985, 1, 119D, (IR)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, 1, 179B; 179C; 180A, (NMR)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, 3, 168A, (IR)

Org. Synth., Coll. Vol., 2, 1943, 317, (合成法)

Lukes, R. et al., Coll. Czech. Chem. Comm., 1960, 25, 483, (絶対構造)

Nigam, N.C. et al., Can. J. Chem., 1964, 42, 2610, (分離)

Zweifel, G. et al., Tet. Lett., 1966, 6021, (合成法)

Carlson, R.M. et al., Tet. Lett., 1971, 3661, (合成法)

Keinan, E. et al., J.A.C.S., 1986, 108, 162, (合成法)

Jolad, S.D. et al., Phytochemistry, 1988, 27, 2199, (分離, 配糖体)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 2, 315

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1267

Sekiwa, Y. et al., Biosci., Biotechnol., Biochem., 1999, 63, 384, (配糖体)

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, HBE500

\*\*\*RTECS (化学物質毒性データ) \*\*\*

\*\*\*健康障害に関するデータ\*\*\*

\*\*\*急性毒性に関するデータ\*\*\*

<<試験方法>> LD50 試験 (50%致死量試験).

曝露経路 : 経口投与.

被験動物 : げっ歯類-ラット.

投与量・期間 : 2580 mg/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参照文献

AMIHBC AMA Archives of Industrial Hygiene and Occupational Medicine. (Chicago, IL) V.2-10, 1950-54. For publisher information, [Vol.,頁,年(19-)] 10,61,1954

<<試験方法>> LD50 試験 (50%致死量試験).

曝露経路 : 皮膚への塗布

被験動物 : げっ歯類-ウサギ.

投与量・期間 : 1780 uL/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参照文献

AMIHBC AMA Archives of Industrial Hygiene and Occupational Medicine. (Chicago, IL) V.2-10, 1950-54. For publisher information, [Vol.,頁,年(19-)] 10,61,1954

\*\*\*米国に於ける状況\*\*\*

EPA TSCA Section 8 (b) CHEMICAL INVENTORY

**§ 2-Heptanol; (±)-form, O-β-D-Glucopyranoside**

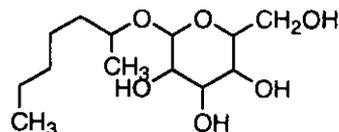
[化合物分類] 脂肪族化合物 (Saturated unbranched alcohol)

[構造式]

[分子量] 278.345

[正確な分子量] 278.17294

[基原] 新鮮なショウガ (*Zingiber officinale*)



-----文献-----

Lukes, R. et al., Coll. Czech. Chem. Comm., 1960, 25, 483, (絶対構造)

Nigam, N.C. et al., Can. J. Chem., 1964, 42, 2610, (分離)

Jolad, S.D. et al., Phytochemistry, 1988, 27, 2199, (分離, 配糖体)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 2, 315

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1267

Sekiwa, Y. et al., Biosci., Biotechnol., Biochem., 1999, 63, 384, (配糖体)

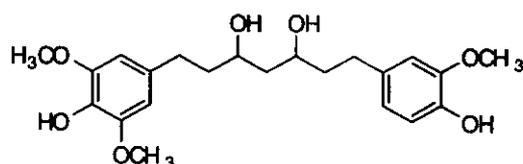
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, HBE500

§ 1-(4-Hydroxy-3,5-dimethoxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)-3,5-heptanediol; (3S,5S)-form

[CAS No.] 145888-84-2

[化合物分類] 単環芳香族 (Diarylalkyl)

[構造式]



[基原] *Zingiber officinale* (ショウガ科) の乾燥根茎

-----文献-----

Yamahara, J. et al., Yakugaku Zasshi, 1992, 112, 645, (分離, 絶対構造)

§ 1-(4-Hydroxy-3-methoxyphenyl)-3-decanone

[化学名・別名] [6]-Paradol. 2-Methoxy-4-(3-oxodecyl) phenol

[CAS No.] 27113-22-0

[化合物分類] 脂肪族化合物 (Long-chain aromatic system)

[構造式]

[分子式] C<sub>17</sub>H<sub>26</sub>O<sub>3</sub>

[分子量] 278.391

[正確な分子量] 278.188195

[基原] grains of paradise (*Amomum melegueta*) とショウガ (*Zingiber officinale*)

[性状] 結晶 (hexane at -30 °C)

[融点] Mp 27-29 °C. Mp 31-32 °C

[化学物質毒性データ総覧 (RTECS) 登録番号] HE0758000

-----文献-----

Connell, D.W., Aust. J. Chem., 1970, 23, 369, (分離, IR, Mass, UV)

Locksley, H.D. et al., J.C.S. Perkin 1, 1972, 3001, (Mass, H-NMR, 合成法)

\*\*\*RTECS (化学物質毒性データ) \*\*\*

生体影響物質 : 医薬品.

\*\*\*健康障害に関するデータ\*\*\*

\*\*\*急性毒性に関するデータ\*\*\*

<<試験方法>> LD50 試験 (50%致死量試験).

曝露経路 : 腹腔内投与

被験動物 : げっ歯類-マウス

投与量・期間 : 270 mg/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参照文献

JTSCDR Journal of Toxicological Sciences. (Japanese Soc. of Toxicological Sciences, 4th Floor, Gakkai Center Bldg., 4-16, Yayoi 2-chome, Bunkyo-ku, Tokyo 113, Japan) V.1- 1976- [Vol.,頁,年(19-)] 16 (Suppl 1), 3,1991

§ Isopropylbenzene (旧 CAS 名)

[化学名・別名] 1-Methylethylbenzene (CAS 名). Cumene. Cumol. 2-Phenylpropane  
[CAS No.] 98-82-8  
[化合物分類] テルペノイド (*p*-Menthane monoterpene) 単環芳香族 (Simple benzene derivative)  
[構造式]  $\text{PhCH}(\text{CH}_3)_2$   
[分子式]  $\text{C}_9\text{H}_{12}$   
[分子量] 120.194  
[正確な分子量] 120.0939  
[基原] ジンジャーオイル (*Zingiber officinale*) の微量成分  
[用途] 麻酔薬. Feedstock for major route for manuf. of Phenol and Acetone via 1-Methyl-1-phenylethyl hydroperoxide. Important industrial chemical, USA production in 1999 3.49 million tons  
[性状] 液体  
[融点]  $Mp$ -96.9 °C  
[沸点]  $Bp$  152-153 °C  
[濃度]  $d^{20}_4$  0.86  
[傷害・毒性] 眼, 唇膜を刺激する. 高濃度蒸気の吸入で麻酔作用を有する. 中枢神経抑制薬. 50 %致死量 ( $LD_{50}$ ) (ラット, 経口) 1400 mg/kg; 50 %致死量 ( $LD_{50}$ ) (ラット, 吸入) 8000 ppm (4 時間暴露)  
[化学物質毒性データ総覧 (RTECS) 登録番号] GR8575000

-----文献-----

Adv. Chem. Ser., 1955, 15, 18, (性質)  
Nigam, M.C. et al., Can. J. Chem., 1964, 42, 2610, (分離)  
Schaefer, T. et al., Can. J. Chem., 1988, 66, 1495, (H-NMR, conformn)  
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, COE750  
Lee, E.W., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1, 1987, 96, (レビュー, 毒性)  
Luxon, S.G., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry, 1992, 348  
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), VNR, 1991, 190  
\*\*\*RTECS (化学物質毒性データ)\*\*\*  
生体影響物質 : 催腫瘍物質 変異原物質. ヒト. 一時刺激物質.  
\*\*\*健康障害に関するデータ\*\*\*  
\*\*\*皮膚/眼の刺激に関するデータ\*\*\*

<<試験方法>> 開放刺激試験  
曝露経路 : 皮膚への塗布  
被験動物 : げっ歯類-ウサギ.  
投与量・期間 : 10 mg/24 時間  
反応の症度 : 中等度.  
参照文献

AMIHBC AMA Archives of Industrial Hygiene and Occupational Medicine. (Chicago, IL) V.2-10, 1950-54. For publisher information, [Vol.,頁,年(19-)]4,119,1951

<<試験方法>> 標準ドライズ試験.  
曝露経路 : 皮膚への塗布  
被験動物 : げっ歯類-ウサギ.  
投与量・期間 : 100 mg/24 時間  
反応の症度 : 軽度  
参照文献

85JCAE "Prehled Prumyslove Toxikologie; Organické Latky," Marhold, J., Prague, Czechoslovakia, Avicenum, 1986 [Vol.,頁,年(19-)]-,33,1986

<<試験方法>> 標準ドライズ試験.  
曝露経路 : 眼中への塗布  
被験動物 : げっ歯類-ウサギ.  
投与量・期間 : 86 mg  
反応の症度 : 中等度.  
参照文献

AMIHAB AMA Archives of Industrial Health. (Chicago, IL) V.11-21, 1955-60. For publisher information, [Vol.,頁,年(19-)]14,387,1956

<<試験方法>> 標準ドライズ試験.  
曝露経路 : 眼中への塗布  
被験動物 : げっ歯類-ウサギ.  
投与量・期間 : 500 mg/24 時間  
反応の症度 : 中等度.  
参考文献

85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague, Czechoslovakia, Avicenum, 1986 [Vol.,頁,年(19-)]-,33,1986

\*\*\*急性毒性に関するデータ\*\*\*

<<試験方法>> 認知されている最小毒性濃度(TCLO)試験.  
曝露経路 : 吸入.  
被験動物 : ヒト  
投与量・期間 : 200 ppm  
毒性影響 : [行動] 傾眠(全身活動度の低下).  
[行動] 抗精神病.  
[行動] 興奮性.

参考文献

TGNCDL "Handbook of Organic Industrial Solvents," 2nd ed., Chicago, National Assoc. of Mutual Casualty Companies, 1961 [Vol.,頁,年(19-)]2,39,1961

<<試験方法>> LD50 試験(50%致死量試験).  
曝露経路 : 経口投与.  
被験動物 : げっ歯類-ラット.  
投与量・期間 : 1400 mg/kg  
毒性影響 : [胃腸] 胃炎.  
参考文献

AMIHAB AMA Archives of Industrial Health. (Chicago, IL) V.11-21, 1955-60. For publisher information, [Vol.,頁,年(19-)]14,387,1956

<<試験方法>> 認知された最小致死濃度(LCLO)に関する試験  
曝露経路 : 吸入.  
被験動物 : げっ歯類-ラット.  
投与量・期間 : 8000 ppm/4 時間  
毒性影響 : 致死量以外に毒性影響に関する報告はない.  
参考文献

AMIHBC AMA Archives of Industrial Hygiene and Occupational Medicine. (Chicago, IL) V.2-10, 1950-54. For publisher information, [Vol.,頁,年(19-)]4,119,1951

<<試験方法>> LD50 試験(50%致死量試験).  
曝露経路 : 経口投与.  
被験動物 : げっ歯類-マウス  
投与量・期間 : 12750 mg/kg  
毒性影響 : 致死量以外に毒性影響に関する報告はない.  
参考文献

GISAAA Gigena i Sanitariya. For English translation, see HYSAAV. (V/O Mezhdunarodnaya Kniga, 113095 Moscow, USSR) V.1- 1936- [Vol.,頁,年(19-)]36(9),18,1971

<<試験方法>> LC50 試験(50%致死濃度試験).  
曝露経路 : 吸入.  
被験動物 : げっ歯類-マウス  
投与量・期間 : 10 gm/m<sup>3</sup>/7 時間  
毒性影響 : [肝臓] 複数の作用.  
[腎臓・尿路・膀胱] 尿細管と糸球体の両方の変化.  
[血液] 脾臓の変化.

参考文献

JHTAB Journal of Industrial Hygiene and Toxicology. (Cambridge, MA) V.18-31, 1936-49. For publisher information, [Vol.,頁,年(19-)]26,264,1944

<<試験方法>> LD50 試験(50%致死量試験).  
曝露経路 : 皮膚への塗布

被験動物 : げっ歯類-ウサギ.  
投与量・期間 : 12300 uL/kg  
毒性影響 : 致死量以外に毒性影響に関する報告はない.  
参照文献

AMIHBC AMA Archives of Industrial Hygiene and Occupational Medicine. (Chicago, IL) V.2-10, 1950-54. For publisher information, [Vol.,頁,年(19-)]4,119,1951

\*\*\*その他の多回投与試験\*\*\*

<<試験方法>> 認知されている最小毒性濃度(TCLO)試験.

曝露経路 : 吸入.  
被験動物 : げっ歯類-ラット.  
投与量・期間 : 1200 ppm/6時間/13週間間欠投与  
毒性影響 : [知覚組織と特異感覚] (眼) その他特定すべき事象なし  
[行動] 活動度の変化(特定の試験).  
[血液] 有色赤血球または有核赤血球.

参照文献

NTIS\*\* National Technical Information Service. (Springfield, VA 22161) Formerly U.S. Clearinghouse for Scientific & Technical Information. [Vol.,頁,年(19-)]OTS0522342

### § 8(17),12-Labdadiene-15,16-diol; (12E)-form, 15,16-Dialdehyde, 8 β,17-Epoxyde

[化学名・別名] 8 β,17-Epoxy-12E-labdene-15,16-dial. ZT

[CAS No.] 71641-23-1

[化合物分類] テルペノイド(Labdane diterpenoid)

[構造式]

[分子式] C<sub>20</sub>H<sub>30</sub>O<sub>3</sub>

[分子量] 318.455

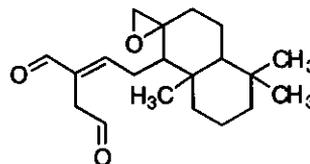
[正確な分子量] 318.219495

[基原] *Aframomum daniellii*, *Zingiber officinale*

[性状] 結晶(C<sub>6</sub>H<sub>6</sub>/petrol)

[融点] Mp 90-92 °C

[比旋光度]: [α]<sub>D</sub> +28.1 (c, 1.41 in CHCl<sub>3</sub>)



-----文献-----

Kimbu, S.F. et al., J.C.S. Perkin 1, 1979, 1303, (epoxide)

Zhou, B.N. et al., J. Nat. Prod., 1997, 60, 1287, (16-Oxolabdadienoic acid)

Ngo, K.S. et al., Phytochemistry, 1998, 47, 1117, (8,17-Epoxy-12-labdene-15,16-dial, H-NMR, C13-NMR)

### § 2-Nonanol(CAS名)(旧CAS名)

[化学名・別名] FEMA 3315

[CAS No.] 628-99-9

[関連CAS No.] 70419-07-7

[その他のCAS No.] 28473-21-4

[化合物分類] 脂肪族化合物(Saturated unbranched alcohol)

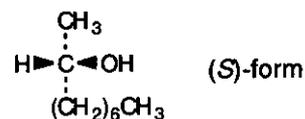
[構造式]

[分子式] C<sub>9</sub>H<sub>20</sub>O

[分子量] 144.256

[正確な分子量] 144.151415

[基原] 色々な精油から分離, 例えば, *Larix laricina*, *Larix lyallii*, *Citrus sinensis*, *Zingiber officinale*, *Anthocephalus cadamba*



-----文献-----

Nair, G.V. et al., Can. J. Chem., 1959, 37, 1608; 1960, 38, 177, (分離)

Keinan, E. et al., J.A.C.S., 1986, 108, 162, (合成法)

Mori, K. et al., Annalen, 1994, 1065, (S-form)

### § Paradol; [8]Paradol, 1,2,4,5-Tetradehydro

[化学名・別名] 1-(4-Hydroxy-3-methoxyphenyl)-1,4-dodecadien-3-one. [8]Dehydroshogaol

[化合物分類] 脂肪族化合物(Long-chain aromatic system), 脂肪族化合物(Branched alkenic aldehydes and

ketone)

[構造式]

[分子式]  $C_{19}H_{26}O_3$

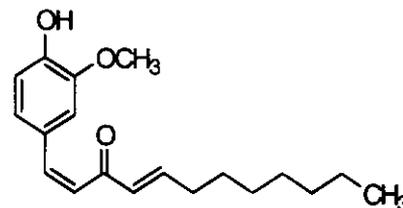
[分子量] 302.413

[正確な分子量] 302.188195

[基原] *Zingiber officinale*

[性状] 黄色のシロップ.

[UV]: [neutral]  $\lambda_{max}$  258 (log  $\epsilon$  3.96); 357 (log  $\epsilon$  4.1) (MeOH)



-----文献-----

Tackie, A.N. et al., *Phytochemistry*, 1975, 14, 853, (分離)

Wu, T.-S. et al., *Phytochemistry*, 1998, 48, 889, (Dehydroshogaol)

§ **Paradol; [10]Paradol, 1,2,4,5-Tetradecydro (E,E-)**

[化学名・別名] 1-(4-Hydroxy-3-methoxyphenyl)-1,4-tetradecadien-3-one. [10]Dehydroshogaol

[化合物分類] 脂肪族化合物 (Branched alkenic aldehydes and ketone), 脂肪族化合物 (Long-chain aromatic system)

[構造式]

[分子式]  $C_{21}H_{30}O_3$

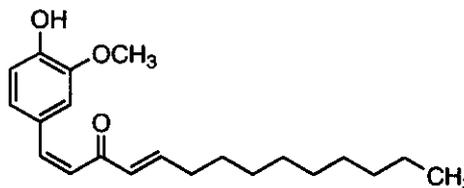
[分子量] 330.466

[正確な分子量] 330.219495

[基原] *Zingiber officinale*

[性状] 黄色のシロップ

[UV]: [neutral]  $\lambda_{max}$  257 (log  $\epsilon$  4.04); 355 (log  $\epsilon$  4.18) (MeOH)



-----文献-----

Wu, T.-S. et al., *Phytochemistry*, 1998, 48, 889, (Dehydroshogaol)

§ **Sesquisabinene;  $\Delta^3$ -Isomer**

[化学名・別名] Sesquithujene

[CAS No.] 58319-06-5

[化合物分類] テルペノイド (Cyclobisabolane sesquiterpenoid)

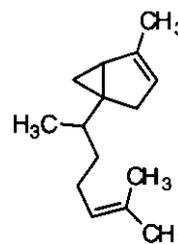
[構造式]

[分子式]  $C_{15}H_{24}$

[分子量] 204.355

[正確な分子量] 204.1878

[基原] 次の植物から分離: *Zingiber officinale*



-----文献-----

Terhune, S.J. et al., *Can. J. Chem.*, 1975, 53, 3285, (分離, 構造決定)

Bohlmann, F. et al., *Phytochemistry*, 1978, 17, 1666, (分離, H-NMR)

Bohlmann, F. et al., *Phytochemistry*, 1982, 21, 1157, (分離, 構造決定)

Sharma, P.K. et al., *Phytochemistry*, 1988, 27, 3471, (合成)

§ **Sesquisabinene; 3,15-Dihydro, 3-hydroxy (cis-)**

[化学名・別名] Sesquisabinene hydrate

[化合物分類] テルペノイド (Cyclobisabolane sesquiterpenoid)

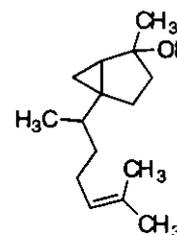
[構造式]

[分子式]  $C_{15}H_{26}O$

[分子量] 222.37

[正確な分子量] 222.198365

[基原] 次の植物の精油から分離: *Zingiber officinale*



-----文献-----

Terhune, S.J. et al., *Can. J. Chem.*, 1975, 53, 3285, (分離, 構造決定)

Bohlmann, F. et al., *Phytochemistry*, 1978, 17, 1666, (分離, H-NMR)

Bohlmann, F. et al., *Phytochemistry*, 1982, 21, 1157, (分離, 構造決定)

Sharma, P.K. et al., *Phytochemistry*, 1988, 27, 3471, (合成)

### § Shogaol; 1,2-Didehydro

[化学名・別名] 1-(4-Hydroxy-3-methoxyphenyl)-1,4-decadien-3-one. [6] Dehydroshogaol

[CAS No.] 212137-55-8

[化合物分類] 脂肪族化合物 (Long-chain aromatic system), 脂肪族化合物 (Branched alkenic aldehydes and ketone)

[構造式]

[分子式]  $C_{17}H_{22}O_3$

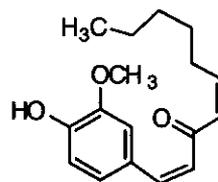
[分子量] 274.359

[正確な分子量] 274.156895

[基原] *Zingiber officinale*

[性状] 黄色のシロップ.

[UV]: [neutral]  $\lambda_{max}$  258 (log  $\epsilon$  3.93); 355 (log  $\epsilon$  4.02) (MeOH)



-----文献-----

Matsushita, Y. et al., Tet. Lett., 1995, 36, 1879, (6-Hydroxysogaol)

Wu, T.-S. et al., Phytochemistry, 1998, 48, 889, (Dehydroshogaol)

Fleming, S.A. et al., Synth. Commun., 1999, 29, 1933, (合成法, H-NMR, C13-NMR)

### § Shogaol; Demethoxy

[化学名・別名] 1-(4-Hydroxyphenyl)-4-decen-3-one. Demethoxysogaol

[CAS No.] 153311-54-7

[化合物分類] 脂肪族化合物 (Branched alkenic aldehydes and ketone), 単環芳香族 (Simple phenol)

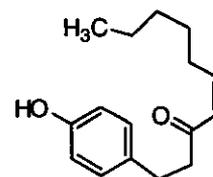
[構造式]

[分子式]  $C_{16}H_{22}O_2$

[分子量] 246.349

[正確な分子量] 246.16198

[基原] *Zingiber officinale*



-----文献-----

Connell, D.W. et al., Aust. J. Chem., 1970, 23, 369, (分離)

Tackre, A.N. et al., Phytochemistry, 1975, 14, 853, (分離)

Matsushita, Y. et al., Tet. Lett., 1995, 36, 1879, (6-Hydroxysogaol)

Wu, T.-S. et al., Phytochemistry, 1998, 48, 889, (Dehydroshogaol)

Fleming, S.A. et al., Synth. Commun., 1999, 29, 1933, (合成法, H-NMR, C13-NMR)

### § Shogaol; 6-Hydroxy

[化学名・別名] 6-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-4-decen-3-one. 6-Hydroxysogaol

[CAS No.] 143114-93-6

[化合物分類] 単環芳香族 (Simple phenol), 脂肪族化合物 (Branched alkenic aldehydes and ketone)

[構造式]

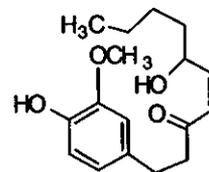
[分子式]  $C_{17}H_{24}O_4$

[分子量] 292.374

[正確な分子量] 292.16746

[基原] *Zingiber officinale*

[比旋光度]:  $[\alpha]_D -1.7$  (c, 1.81 in  $CHCl_3$ )



-----文献-----

Connell, D.W. et al., Aust. J. Chem., 1970, 23, 369, (分離)

Tackre, A.N. et al., Phytochemistry, 1975, 14, 853, (分離)

Banno, K. et al., Bull. Chem. Soc. Jpn., 1976, 49, 1453, (合成法)

Chen, C.C. et al., J. Chromatogr., 1986, 360, 175

Vig, O.P. et al., Indian J. Chem., Sect. B, 1990, 29, 284, (合成法)

Hatanaka, M. et al., J.O.C., 1994, 59, 111, (合成法)

Matsushita, Y. et al., Tet. Lett., 1995, 36, 1879, (6-Hydroxysogaol)

Wu, T.-S. et al., Phytochemistry, 1998, 48, 889, (Dehydroshogaol)

Fleming, S.A. et al., Synth. Commun., 1999, 29, 1933, (合成法, H-NMR, C13-NMR)

\*\*\*\*\*シヨウユ (Soy sauce) \*\*\*\*\*

§ § 醤油または醤油もろみ。

\*\*\*\*\*シヨウユカス (Pressed soy sauce cake) \*\*\*\*\*

§ § 醤油粕。

\*\*\*\*\*ジヨウリュウシュ (Spirits) \*\*\*\*\*

§ § ラム, ウイスキー, ジン, ブランデー, チェリーブランデー (キルシュパッサー), アップル  
ブランデー, アプリコットブランデー, アワモリ, 焼酎などの蒸留酒。

\*\*\*\*\*シヨウロ (Shoro) \*\*\*\*\*

§ § ヒメノガステル科シヨウロ (*Rhizopogon rubescens* Tul.) の子実体。  
本調査研究では研究報告ない。

\*\*\*\*\*シルバーウィード (Silver weed) \*\*\*\*\*

§ § パラ科ヨウシュツルキンバイ (*Potentilla anserina* L.) の根、葉又 H 全草。  
本調査研究では研究報告ない。

\*\*\*\*\*シロタモギタケ (Elm-mushroom) \*\*\*\*\*

§ § シメジ科シロタモギタケ (ブナシメジ) (*Lyophyllum ulmarium* (Fr.) Kuhner.) の子実 体。

§ 2-Amino-3,4-dihydroxybutanoic acid; (2R,3R)-form

[化学名・別名] (+)-*threo*-form. 2-Amino-3,4-dihydroxythreonic acid

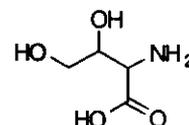
[CAS No.] 21768-44-5

[構造式]

[基原] 次の植物から分離: *Lyophyllum ulmarium*

[融点] Mp 214-215 °C (194 °C)

[比旋光度]:  $[\alpha]_D^{25} +13.6$  (c, 4.8 in H<sub>2</sub>O)



-----文献-----

Niemann, C. et al., J. Biol. Chem., 1942, 143, 191, (合成法)

Hamel, E.E. et al., J.A.C.S., 1953, 75, 1362, (構造)

Okawa, K. et al., Bull. Chem. Soc. Jpn., 1969, 42, 2720, (分割)

Westley, J.W. et al., J. Antibiot., 1971, 24, 330, (分離)

Katz, E. et al., J. Antibiot., 1974, 27, 952

Ogawa, T. et al., Phytochemistry, 1984, 23, 684; 1985, 24, 1837, (分離)

Pirung, M.C. et al., Bioorg. Med. Chem. Lett., 1993, 3, 2095, (合成法, 絶対構造)

Cativiela, C. et al., Tetrahedron, 1996, 52, 9563, (合成法)

§ 2-Amino-3,4-dihydroxybutanoic acid; (2R,3R)-form, 4-Et ether

[化学名・別名] 2-Amino-4-ethoxy-3-hydroxybutanoic acid

[CAS No.] 98644-37-2

[化合物分類] アミノ酸とペプチド (Non-protein  $\alpha$ -aminoacid)

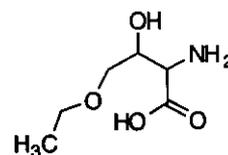
[構造式]

[分子式]  $C_6H_{13}NO_4$

[分子量] 163.173

[正確な分子量] 163.084459

[基原] 次の植物から分離: マッシュルーム *Lyophyllum ulmarium*



-----文献-----

Niemann, C. et al., J. Biol. Chem., 1942, 143, 191, (合成法)

Hamel, E.E. et al., J.A.C.S., 1953, 75, 1362, (構造)

Okawa, K. et al., Bull. Chem. Soc. Jpn., 1969, 42, 2720, (分割)

Westley, J.W. et al., J. Antibiot., 1971, 24, 330, (分離)

Katz, E. et al., J. Antibiot., 1974, 27, 952

Ogawa, T. et al., Phytochemistry, 1984, 23, 684; 1985, 24, 1837, (分離)

Pirung, M.C. et al., Bioorg. Med. Chem. Lett., 1993, 3, 2095, (合成法, 絶対構造)

Cativiela, C. et al., Tetrahedron, 1996, 52, 9563, (合成法)

\*\*\*\*\*ジンセン (Ginseng) \*\*\*\*\*

§ § ウコギ科チヨウセンニンジン (*Panax ginseng* C.A. Meyer) の根。

§ Benzyl alcohol; *O*-[ $\beta$ -D-Xylopyranosyl-(1  $\rightarrow$  6)-D-glucopyranoside]

[化学名・別名] Benzyl  $\beta$ -primeveroside

[CAS No.] 130622-31-0

[化合物分類] 単環芳香族 (Simple benzyl alcohol)

[構造式]

[分子式]  $C_{18}H_{26}O_{10}$

[分子量] 402.397

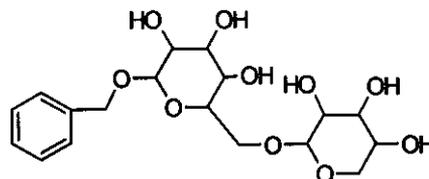
[正確な分子量] 402.1526

[基原] *Alangium platanifolium*, *Camellia sinensis*, *Panax ginseng*, *Prunus laurocerasus*

[性状] 結晶 (EtOH)

[融点] Mp 188-189 °C

[比旋光度]:  $[\alpha]_D^{20}$  -71.2 (c, 1 in H<sub>2</sub>O)



-----文献-----

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaeuser Verlag, Basel, 1972, no. 248, (生育)

Opdyke, D.L.J., Food Cosmet. Toxicol., 1973, 11, 1011, (レビュー, 毒性)

Guo, W. et al., Biosci., Biotechnol., Biochem., 1994, 58, 1532, (primeveroside)

Luxon, S.G., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry, 1992, 120; 121

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, BDX500

§ 10-Chloro-1,16-heptadecadiene-4,6-diyne-3,9-diol

[化学名・別名] Ginsenoyne B

[CAS No.] 139035-29-3

[化合物分類] 脂肪族化合物 (Acetylenic alcohol),

[構造式]  $H_2C=CHCH(OH)C \equiv CC \equiv CCH_2CH(OH)CHCl(CH_2)_3CH=CH_2$

[分子式]  $C_{17}H_{27}ClO_2$

[分子量] 294.82

[正確な分子量] 294.138657

[基原] 次の植物の根から分離: *Panax ginseng*

[性状] オイル

[比旋光度]:  $[\alpha]_D$  -33 (c, 2.0 in  $CHCl_3$ )

[UV]: [neutral]  $\lambda_{max}$  201 ; 230 ; 243 ; 257 ( $CHCl_3$ )

-----文献-----