

[融点] Mp 190-192 °C

-----文献-----

Kimura, Y. et al., Agric. Biol. Chem., 1974, 38, 1507, (2-malonylaminobenzoic acid)

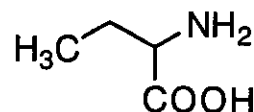
§ 2-Aminobutanoic acid; (R)-form

[化学名・別名] D-form

[CAS No.] 2623-91-8

[化合物分類] アミノ酸とペプチド (Non-protein α -aminoacids)

[構造式]



[分子式] C₄H₉NO₂

[分子量] 103.121

[基原] *Glycine max* の種子, *Dolichos lablab*, *Canavalia gladiata*, *Arachis hypogaea*, *Pisum sativum*, *Phaseolus vulgaris* と *Vigna sesquipedalis* の加水分解後の物質

[性状] 葉状結晶 (EtOH 溶液)

[融点] Mp 292 °C で分解

[比旋光度]: $[\alpha]_D^{20}$ -7.86 (H₂O) (5 M HCl)

[販売元] Aldrich:11612-2; Fluka:7210; Sigma:A1629

-----文献-----

Akimoto, T. et al., Acta Cryst. B, 1972, 28, 3106, (結晶構造)

Ogawa, T. et al., Agric. Biol. Chem., 1976, 40, 1661, (生育)

Glowiak, T. et al., Bull. Acad. Pol. Sci., Ser. Sci. Chim., 1978, 26, 43, (結晶構造)

Chenault, H.K. et al., J.O.C., 1987, 52, 2608, (分割, H-NMR)

§ 4-Amino-2-methylenebutanoic acid (CAS 名)

[化学名・別名] γ -Amino- α -methylenebutyric acid

[CAS No.] 65370-67-4

[化合物分類] アミノ酸とペプチド (Unsaturated aminoacids), アミノ酸とペプチド (β -Aminoacids)

[構造式] H₂C=C(COOH)CH₂CH₂NH₂

[分子式] C₅H₉NO₂

[分子量] 115.132

[基原] *Arachis hypogaea*

[性状] 結晶 (EtOH 溶液 or EtOH/Me₂CO)

[融点] Mp 152 °C で分解. Mp 170-179 °C で分解

-----文献-----

Fowden, L. et al., Biochem. J., 1953, 55, 548

Marcus, A. et al., Arch. Biochem. Biophys., 1963, 100, 80

Hatanaka, S. et al., Phytochemistry, 1977, 16, 1820, (合成法, NMR)

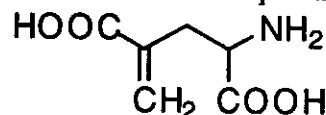
§ 2-Amino-4-methylenepentanedioic acid; (S)-form

[化学名・別名] L-form

[CAS No.] 16804-57-2

[化合物分類] アミノ酸とペプチド (Unsaturated aminoacids), アミノ酸とペプチド (Non-protein α -aminoacids)

[構造式]



[分子式] C₆H₉NO₄

[分子量] 159.141

[基原] ピーナッツ (*Arachis hypogaea*), その他の植物, notably tulips and hops. 次の植物から分離: シダ類 *Asplenium* spp., *Phyllitis scolopendrium*

[比旋光度]: $[\alpha]_D^{20}$ +13.7 (5 M HCl)

[販売元] Sigma:M2879

-----文献-----

Virtanen, A.I. et al., Acta Chem. Scand., 1955, 9, 553, (分離)

Marcus, A. et al., Arch. Biochem. Biophys., 1963, 100, 80, (合成法)

Blake, J. et al., Biochem. J., 1964, 92, 136, (分離, 絶対構造)

Meier, L.K. et al., Phytochemistry, 1979, 18, 1173, (分離)

Moody, C.M. et al., J.C.S. Perkin 1, 1997, 3519-3530, (合成法, IR, H-NMR, C13-NMR)

§ Arachidin I; (E,E)-form

[CAS No.] 98391-38-9

[化合物分類] 単環芳香族 (Stilbenes)

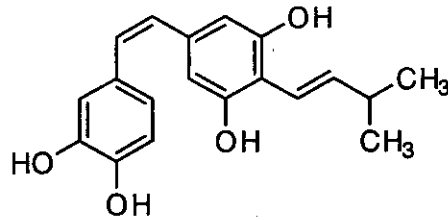
[構造式]

[分子式] $C_{19}H_{20}O_4$

[分子量] 312.365

[基原] ピーナッツ (*Arachis hypogaea*)

[用途] ファイトアレキシン



-----文献-----

Keen, N.T. et al., *Phytochemistry*, 1976, 15, 1794, (分離)

Aguamah, G.E. et al., *Phytochemistry*, 1981, 20, 1381, (分離)

Wotton, H.R. et al., *J. Gen. Microbiol.*, 1985, 131, 487, (分離)

Boonlaksiri, C. et al., *Phytochemistry*, 2000, 54, 415-417, (3'-Deoxy-2'-hydroxy)

§ Arachidin I; (E,E)-form, 3'-Deoxy

[化学名・別名] 5-[2-(4-Hydroxyphenyl) ethenyl]-2-(3-methyl-1-butenyl)-1,3-benzenediol (CAS 名). 3,4,5-Trihydroxy-4-(3-methyl-1-butenyl) stilbene. Arachidin III

[CAS No.] 87320-15-8

[化合物分類] 単環芳香族 (Stilbenes)

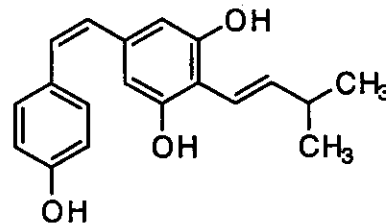
[構造式]

[分子式] $C_{19}H_{20}O_3$

[分子量] 296.365

[基原] 次の植物から分離: *Arachis hypogaea*

[用途] ファイトアレキシン



-----文献-----

Keen, N.T. et al., *Phytochemistry*, 1976, 15, 1794, (分離)

Aguamah, G.E. et al., *Phytochemistry*, 1981, 20, 1381, (分離)

Wotton, H.R. et al., *J. Gen. Microbiol.*, 1985, 131, 487, (分離)

Boonlaksiri, C. et al., *Phytochemistry*, 2000, 54, 415-417, (3'-Deoxy-2'-hydroxy)

§ Arachidin II; (E)-form

[CAS No.] 61517-87-1

[化合物分類] 単環芳香族 (Stilbenes)

[構造式]

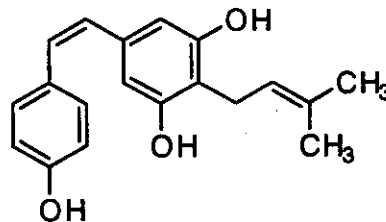
[分子式] $C_{19}H_{20}O_3$

[分子量] 296.365

[基原] ピーナッツ (*Arachis hypogaea*)

[用途] ファイトアレキシン

[性状] 黄色のオイル



-----文献-----

Braz Filho, R. et al., *Phytochemistry*, 1975, 14, 1454, (誘導体)

Keen, N.T. et al., *Phytochemistry*, 1976, 15, 1794, (分離)

Takasugi, M. et al., *Chem. Lett.*, 1978, 1241-1242, (2',3,4',5'-Tetrahydroxy-4-prenylstilbene)

Aguamah, G.E. et al., *Phytochemistry*, 1981, 20, 1381, (分離)

Magalhaes, A.F. et al., *Phytochemistry*, 2001, 57, 77-89, (3,5-di-Me ether)

§ Arachidoside

[化合物分類] フラボノイド (Flavonoids 構造は一部又は全てが未知)

[一般的性質] 構造は未知. フラボノイド配糖体. Poss. a glycoside of Dihydroisorhamnetin (3,3',4',5,7-Pentahydroxyflavanone 参照)

[基原] 次の植物から分離: ピーナッツ (*Arachis hypogaea*) の殻

[性状] 茶-赤色の粉末

-----文献-----

Tuyeau, F. et al., *C. R. Hebd. Seances Acad. Sci.*, 1947, 224, 290

§ 3,5-Dihydroxybenzoic acid (CAS 名)

[化学名・別名] α -Resorcylic acid (旧 CAS 名). Resorcinol-5-carboxylic acid

[CAS No.]99-10-5

[関連 CAS No.]41696-97-3

[化合物分類]PS7950, 単環芳香族 (Simple benzoic acids and esters), PA2000

[構造式]構造式は次の化合物と類似: 2,3-Dihydroxybenzoic acid

[分子式]C₇H₆O₄

[分子量]154.122

[基原]*Arachis hypogaea* と *Cicer arietinum* の種子. また *Pterocarpus santalinus* にも存在する

[性状]結晶+ 1·1/2H₂O (H₂O)

[融点]Mp 232-233 °C (無水物)

[溶解性]水に可溶

[PKa 値]pK_a 4.04

[化学物質毒性データ総覧 (RTECS) 登録番号]VH3708000

[販売元]Aldrich:D11000-0; Fluka:37600; Sigma:R1500

-----文献-----

Hawker, C.J. et al., J.C.S. Perkin 1, 1992, 2459, (dendritic polyesters)

Chakraborty, T.K. et al., J.O.C., 1992, 57, 5462, (Me esters)

Walpole, C.S.J. et al., J. Med. Chem., 1993, 36, 2362, (Mono-Me ether, nitrile)

Zhu, J. et al., J.O.C., 1995, 60, 6389, (誘導体, 合成法, H-NMR, C13-NMR)

McElhanon, J.R. et al., J.O.C., 1997, 62, 908-915, (Dibenzyl ether Me ester)

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 : 静脈内投与.

被験動物 : げっ歯類-マウス.

投与量・期間 : 2 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.

参考文献

Progress in Medical Chemistry. (Elsevier Science Pub. Co., Inc., 52 Vanderbilt Ave., New York, NY 10017) 5,59,1967

§ 5,7-Dihydroxyisoflavone (旧 CAS 名)

[化学名・別名]5,7-Dihydroxy-3-phenyl-4H-1-benzopyran-4-one (CAS 名)

[CAS No.]4044-00-2

[化合物分類]フラボノイド (Isoflavones; 2 × O-置換基)

[構造式]

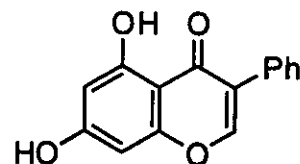
[分子式]C₁₅H₁₀O₄

[分子量]254.242

[基原]次の植物から分離: hydrolysed flour of *Arachis hypogaea* (ピーナッツ)

[性状]針状結晶 (EtOH 溶液)

[融点]Mp 205 °C (195-196 °C)



-----文献-----

Audier, H., Bull. Soc. Chim. Fr., 1966, 2892, (Mass)

Daigle, D.J. et al., CA, 1986, 104, 165440, (分離)

Murthy, M.S.R. et al., Magn. Reson. Chem., 1986, 24, 225, (C13-NMR)

§ 5,7-Dihydroxyisoflavone; Di-Me ether

[化学名・別名]5,7-Dimethoxyisoflavone

[CAS No.]26964-35-2

[化合物分類]フラボノイド (Isoflavones; 2 × O-置換基)

[構造式]

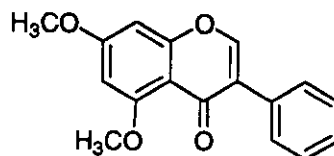
[分子式]C₁₇H₁₄O₄

[分子量]282.295

[基原]次の植物から分離: *Cordyla africana* の心材, *Arachis hypogaea* の種子

[性状]板状結晶 (EtOH 溶液)

[融点]Mp 122-123 °C (112 °C)



-----文献-----

Audier, H., Bull. Soc. Chim. Fr., 1966, 2892, (Mass)
Daigle, D.J. et al., CA, 1986, 104, 165440, (分離)
Murthy, M.S.R. et al., Magn. Reson. Chem., 1986, 24, 225, (C13-NMR)

§ 1-(3,5-Dihydroxyphenyl)-2-(4-hydroxyphenyl) ethylene; (E)-form

[CAS No.] 501-36-0

[化合物分類] 単環芳香族 (Stilbenes)

[構造式]

[分子式] $C_{14}H_{12}O_3$

[分子量] 228.247

[基原] 次の植物のファイトアレキシン: *Veratrum grandiflorum* (根), *Pinus sibirica* (樹皮), *Vitis vinifera*, *Arachis hypogaea*. また *Eucalyptus*, *Polygonum*, *Nothofagus* spp., *Cudrania javanensis* から得られる

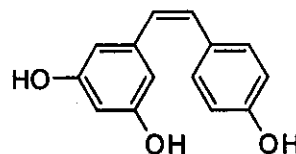
[用途] Fungicide, bactericide. Resveratrol in red wines has been postulated to be associated with beneficial health effects. Shows Tyrosinase inhibitory activity

[性状] 結晶 (MeOH 溶液)

[融点] Mp 265-267 °C

UV: [neutral] λ_{max} 218 (ϵ 21400); 227 (sh) (ϵ 14800); 307 (ϵ 27500); 320 (ϵ 26900) (EtOH)

[販売元] Sigma:R5010



----- 文献 -----

Banks, H.J. et al., Aust. J. Chem., 1971, 24, 2427, (分離, 誘導体)
Murakami, T. et al., Tet. Lett., 1972, 2965, (分離, UV)
Kumar, N. et al., Phytochemistry, 1974, 13, 633, (分離)
Sotheeswaran, S. et al., Phytochemistry, 1993, 32, 1083, (レビュー, 成書)

§ 1-(3,5-Dihydroxyphenyl)-2-(4-hydroxyphenyl) ethylene; (Z)-form

[CAS No.] 61434-67-1

[化合物分類] 単環芳香族 (Stilbenes)

[構造式]

[分子式] $C_{14}H_{12}O_3$

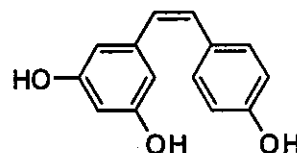
[分子量] 228.247

[基原] 次の植物から得られるファイトアレキシン: *Arachis hypogaea*

[性状] 粉末 (MeOH 溶液)

[融点] Mp 170-174 °C

UV: [neutral] λ_{max} 210; 220 (sh); 286 (EtOH)



----- 文献 -----

Banks, H.J. et al., Aust. J. Chem., 1971, 24, 2427, (分離, 誘導体)
Murakami, T. et al., Tet. Lett., 1972, 2965, (分離, UV)
Kumar, N. et al., Phytochemistry, 1974, 13, 633, (分離)
Aritomi, M. et al., Phytochemistry, 1976, 15, 2006, (分離, UV)
Nonaka, G.-I. et al., Chem. Pharm. Bull., 1977, 25, 2300, (分離, UV, IR, H-NMR, 誘導体)
Nakajima, K. et al., Chem. Pharm. Bull., 1978, 26, 3050, (分離, IR, UV, H-NMR)
Sotheeswaran, S. et al., Phytochemistry, 1993, 32, 1083, (レビュー, 成書)
Jayatilake, G.S. et al., J. Nat. Prod., 1995, 58, 1958, (分離, triacetate, H-NMR, C13-NMR)

§ 1,12-Dodecanediol; Di-Ph ether

[化学名・別名] 1,1'-[1,12-Dodecanediylbis(oxy)] bisbenzene (CAS 名).

1,12-Diphenoxydodecane

[CAS No.] 61575-03-9

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

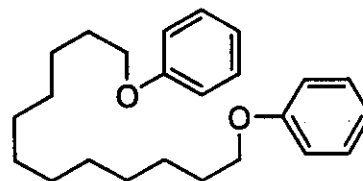
[構造式]

[分子式] $C_{24}H_{42}O_2$

[分子量] 354.531

[基原] 次の植物から分離: *Puccinia arachidis* に感染した *Arachis hypogaea* の葉

[用途] ファイトアレキシン



----- 文献 -----

Rosen, M.J. et al., J. Am. Oil Chem. Soc., 1976, 53, 742, (di-Ph ether)
Rao, P.V.S. et al., Oleagineux, 1991, 46, 501; CA, 116, 252152, (di-Ph ether)

Nakamura, N. et al., Acta Cryst. C, 1997, 53, 1883-1885, (結晶構造)

§ Eicosanoic acid

[化学名・別名] Arachidic acid. Icosanoic acid. Arachic acid

[CAS No.] 506-30-9

[関連 CAS No.] 14923-81-0

[化合物分類] 脂肪族化合物 (Saturated unbranched carboxylic acids and lactones)

[構造式] $\text{H}_3\text{C}(\text{CH}_2)_{18}\text{COOH}$

[分子式] $\text{C}_{20}\text{H}_{40}\text{O}_2$

[分子量] 312.535

[基原] arachis (*Arachis hypogaea*) (ground-nut) oil glycerides. その他の種子オイルに広く分布する

[性状] 結晶 (EtOH)

[融点] Mp 77 °C

[沸点] Bp, 203-205 °C

[溶解性] BERDY SOL: クロロホルム, ヘキサンに可溶; 水に難溶

[化学物質毒性データ総覧 (RTECS) 登録番号] JX3780000

[販売元] Aldrich:E23-1; Fluka:10933; Sigma:A3631

----- 文 献 -----

Radler, F. et al., Aust. J. Chem., 1965, 18, 1059, (分離)

Marosi, L. et al., Annalen, 1973, 584, (性質, 結晶構造)

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, EAF000

***RTECS (化学物質毒性データ) ***

生体影響物質 : 催腫瘍物質.

健康障害に関するデータ

催腫瘍性に関するデータ

<<試験方法>> 最小毒性量 (TDLo).

曝露経路 : 埋め込み.

被験動物 : げっ歯類-マウス.

投与量・期間 : 1000 mg/kg

毒性影響 : [催腫瘍性] RTECS 基準による催腫瘍性.

[腎臓・尿路・膀胱] 腫瘍.

参考文献

Cancer Research. (Public Ledger Building, Suit 816, 6th & Chestnut Sts., Philadelphia, PA 19106) 26,105,1966

§ 2-Hexanone (CAS 名)

[化学名・別名] Butyl methyl ketone. Methyl butyl ketone

[CAS No.] 591-78-6

[化合物分類] 脂肪族化合物 (Saturated unbranched aldehydes and ketones)

[構造式] $\text{H}_3\text{C}(\text{CH}_2)_3\text{COCH}_3$

[分子式] $\text{C}_6\text{H}_{12}\text{O}$

[分子量] 100.16

[基原] ホップオイル (*Humulus lupulus*), ポテト (*Solanum tuberosum*), アメリカホドイモ (*Arachis hypogaea*) に存在

[性状] 液体

[沸点] Bp 127 °C

[濃度] d_4^{20} 0.83

[傷害・毒性] 発火しやすい, 発火温度: 23 °C, 自然発火温度: 423 °C. 眼と皮膚を刺激する. 慢性の暴露は末梢の神経症に発展する. 早い時期に頭痛と悪心が現れる. 50 % 致死量 (LD_{50}) (ラット, 経口) 2590 mg/kg. OES: long-term 5 ppm (Sk)

[化学物質毒性データ総覧 (RTECS) 登録番号] MP1400000

[販売元] Aldrich:10300-4; Fluka:20270; Supelco:R43-4110

----- 文 献 -----

Wagner, G., J. Prakt. Chem., 1891, 44, 259

Grignard, V. et al., C. R. Hebd. Seances Acad. Sci., 1926, 182, 299

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1104

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, HEV000

Luxon, S.G., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry, 1992, 672

§ 1- [4-Hydroxy-3-(3-methyl-1,3-butadienyl) phenyl]-2-(3,5-dihydroxyphenyl) ethylene; (E)-form

[化合物分類] 単環芳香族 (Stilbenes)

[構造式]

[分子式] $C_{19}H_{18}O_3$

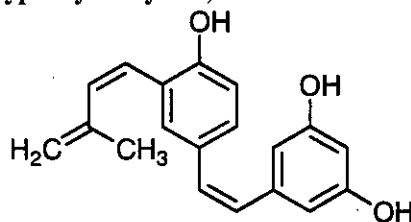
[分子量] 294.344

[基原] *Arachis hypogaea*

[用途] Antifungal phytoalexin

UV: [neutral] λ_{max} 298 (ϵ 22000) (MeOH) (Berdy) [neutral] λ_{max}

296 (EtOH) (Berdy) [base] λ_{max} 341 (MeOH-NAOH) (Berdy)



-----文献-----

Cooksey, C.J. et al., Phytochemistry, 1988, 27, 1015

§ 2-Methylene-4-oxopentanedioic acid

[化学名・別名] γ -Methylene- α -ketoglutaric acid. 2-Methylene-4-oxoglutaric acid

[化合物分類] 脂肪族化合物 (Branched alkenic carboxylic acids)

[構造式] $H_2C=C(COOH)CH_2COCOOH$

[分子式] $C_6H_6O_5$

[分子量] 158.11

[基原] 次の植物から分離: *Tulipa gesneriana* の葉, *Arachis hypogaea*. 次の植物にも僅かに存在する: *Sophora japonica*

-----文献-----

Towers, G.H.N. et al., J.A.C.S., 1954, 76, 1959

Fowden, L. et al., Biochem. J., 1955, 59, 228

Winter, H.C. et al., Phytochemistry, 1987, 26, 2477, (生育)

§ 2-Oxo-4-methylenepentanedioic acid

[化学名・別名] α -Keto- γ -methyleneglutamic acid

[CAS No.] 55601-65-5

[化合物分類] 脂肪族化合物 (Unbranched alkenic carboxylic acids and lactones)

[構造式] $H_2C=C(COOH)CH_2COCOOH$

[分子式] $C_6H_6O_5$

[分子量] 158.11

[基原] Found in tulip *Tulipa gesneriana*, *Lilium* spp. and ground nut (*Arachis hypogaea*)

-----文献-----

Towers, G.H.N. et al., J.A.C.S., 1954, 76, 1959

Fowden, L. et al., Biochem. J., 1955, 59, 228

§ 3,3',4',5,7-Pentahydroxyflavan (2 \rightarrow 7,4 \rightarrow 6)-3,3',4',5,7-pentahydroxyflavan; (2R,2'R,3R,3'S,4R)-form

[化学名・別名] Epicatechin-(2 β \rightarrow 7,4 β \rightarrow 6)-catechin

[化合物分類] フラボノイド (Proanthocyanidin flavonoids)

[構造式]

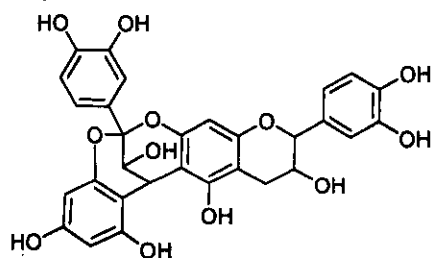
[分子式] $C_{30}H_{26}O_{12}$

[分子量] 576.512

[基原] ピーナッツ (*Arachis hypogaea*) の皮

[性状] 針状結晶・一水和物 (H_2O)

[融点] Mp 271-273 $^{\circ}C$ で分解



-----文献-----

Morimoto, S. et al., Chem. Pharm. Bull., 1987, 35, 4717

Lou, H. et al., Phytochemistry, 1999, 51, 297-308, (分離, CD, H-NMR, C13-NMR)

Kamiya, K. et al., Chem. Pharm. Bull., 2001, 49, 551-557, (Proanthocyanidin A 6, 分離, H-NMR, C13-NMR)

§ 3,3',4',5,7-Pentahydroxyflavan (2 \rightarrow 7,4 \rightarrow 6)-3,3',4',5,7-pentahydroxyflavan; (2R,2'S,3R,3'R,4R)-form

[化学名・別名] Epicatechin-(2 β →7,4 β →6)-*ent*-catechin

[化合物分類] フラボノイド (Proanthocyanidin flavonoids)

[構造式]

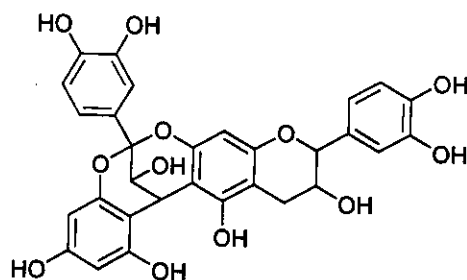
[分子式] C₃₀H₂₄O₁₂

[分子量] 576.504

[基原] ピーナッツ (*Arachis hypogaea*) の皮

[性状] 無定型の粉末・二水和物 (H₂O)

[融点] Mp 262 °C



-----文献-----

Morimoto, S. et al., Chem. Pharm. Bull., 1987, 35, 4717

Lou, H. et al., Phytochemistry, 1999, 51, 297-308, (分離, CD, H-NMR, C13-NMR)

Kamiya, K. et al., Chem. Pharm. Bull., 2001, 49, 551-557, (Proanthocyanidin A 6, 分離, H-NMR, C13-NMR)

§ 3,3',4',5,7-Pentahydroxyflavan(2→7,4→6)

-3,3',4',5,7-pentahydroxyflavan; (2*R*,2'*S*,3*R*,3'*S*,4*R*)-form

[化学名・別名] Epicatechin-(2 β →7,4 β →6) *ent*-catechin

[化合物分類] フラボノイド (Proanthocyanidin flavonoids)

[構造式]

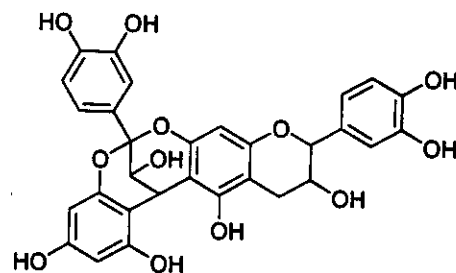
[分子式] C₃₀H₂₄O₁₂

[分子量] 576.512

[基原] ピーナッツ (*Arachis hypogaea*) の皮

[性状] 無定型の粉末・二水和物 (H₂O)

[融点] Mp 280 °Cで分解



-----文献-----

Morimoto, S. et al., Chem. Pharm. Bull., 1987, 35, 4717

Lou, H. et al., Phytochemistry, 1999, 51, 297-308, (分離, CD, H-NMR, C13-NMR)

Kamiya, K. et al., Chem. Pharm. Bull., 2001, 49, 551-557, (Proanthocyanidin A 6, 分離, H-NMR, C13-NMR)

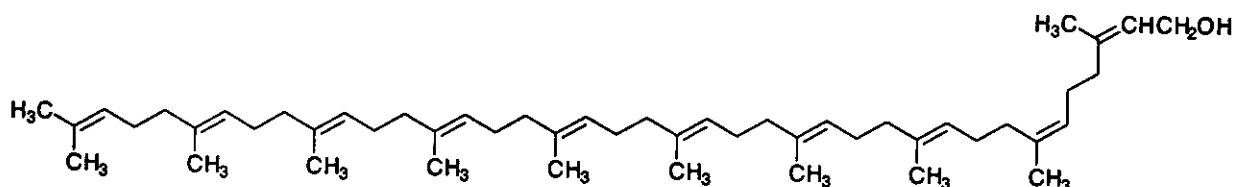
§ Polyprenol; Betulaprenol 10, (2*Z*,6*Z*,10*Z*,14*Z*,18*Z*,22*Z*,26*Z*,30*Z*)-isomer

[化学名・別名] Arachisprenol 10

[化合物分類] テルペノイド

(Polyterpenoids)

[構造式]



[分子式] C₅₀H₈₂O

[分子量] 699.197

[基原] *Arachis hypogaea*

[性状] オイル

-----文献-----

Morton, R.A., Biochem. J., 1972, 128, 11P, (レビュー)

Barrero, A.F. et al., J. Nat. Prod., 1997, 60, 65, (Betulaprenol 6, H-NMR, C13-NMR)

Aoki, T. et al., Phytochemistry, 1997, 46, 715-720, (Arachisprenols, Glycinoprenols 7 and 8)

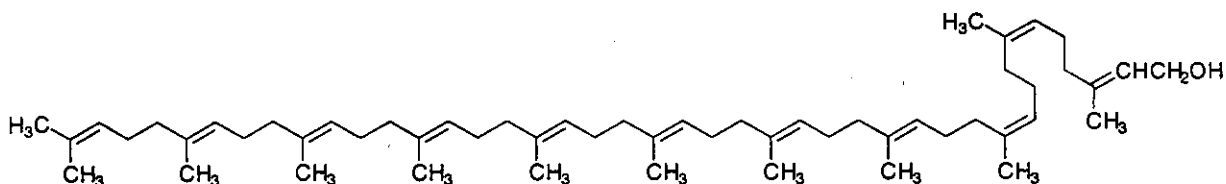
Costantino, V. et al., Tetrahedron, 2000, 56, 1393-1395, (Plakopolyprenoside)

§ Polyprenol; Betulaprenol 11, (2*Z*,6*Z*,10*Z*,14*Z*,18*Z*,22*Z*,26*Z*,30*Z*,34*Z*)-isomer

[化学名・別名] Arachisprenol 11

[化合物分類] テルペノイド (Polyterpenoids)

[構造式]



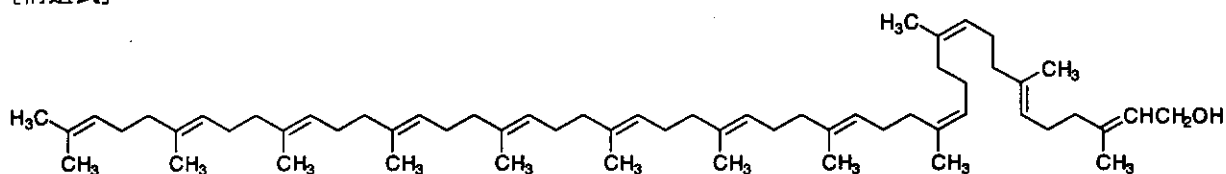
[分子式] $C_{55}H_{90}O$
 [分子量] 767.315
 [基原] *Arachis hypogaea*
 [性状] オイル

----- 文 献 -----

Aoki, T. et al., *Phytochemistry*, 1997, 46, 715-720, (Arachisprenenols, Glycinoprenols 7 and 8)
 Costantino, V. et al., *Tetrahedron*, 2000, 56, 1393-1395, (Plakopolyprenoside)

§ **Polyprenol; Betulaprenol 12, (2Z,6Z,10Z,14Z,18Z,22Z,26Z,30Z,34Z,38Z) -isomer**

[化学名・別名] Arachisprenenol 12
 [化合物分類] テルペノイド (Polyterpenoids)
 [構造式]



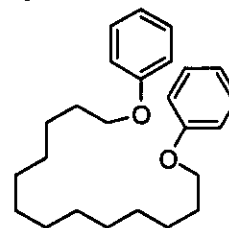
[分子式] $C_{60}H_{98}O$
 [分子量] 835.434
 [基原] *Arachis hypogaea*
 [性状] オイル

----- 文 献 -----

Aoki, T. et al., *Phytochemistry*, 1997, 46, 715-720, (Arachisprenenols, Glycinoprenols 7 and 8)

§ **1,13-Tridecanediol; Di-Ph ether**

[化学名・別名] 1,1'-[1,13-Tridecanediylbis (oxy)] bisbenzene (CAS 名). 1,13-Diphenoxytridecane
 [CAS No.] 141620-05-5
 [化合物分類] 脂肪族化合物 (Saturated unbranched alcohols)
 [構造式]
 [分子式] $C_{25}H_{36}O_2$
 [分子量] 368.558
 [基原] 次の植物から分離: *Puccinia arachidis* に感染した *Arachis hypogaea* の葉
 [用途] ファイトアレキシン

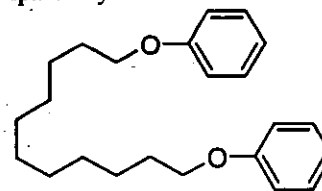


----- 文 献 -----

Rao, P.V.S. et al., *Oleagineux*, 1991, 46, 501; *CA*, 116, 252152, (di-Ph ether)
 Nakamura, N. et al., *Acta Cryst. C*, 1997, 53, 253-255, (結晶構造)

§ **1,11-Undecanediol; Di-Ph ether**

[化学名・別名] 1,1'-[1,11-Undecanediylbis (oxy)] bisbenzene (CAS 名). 1,11-Diphenoxyundecane
 [CAS No.] 141620-04-4
 [化合物分類] 脂肪族化合物 (Saturated unbranched alcohols)
 [構造式]
 [分子式] $C_{23}H_{32}O_2$
 [分子量] 340.505
 [基原] 次の植物から分離: *Puccinia arachidis* に感染した *Arachis hypogaea* の葉
 [用途] ファイトアレキシン



----- 文 献 -----

Rao, P.V.S. et al., *Oleagineux*, 1991, 46, 501; *CA*, 116, 252152, (di-Ph ether)
 Gawarikar, R. et al., *Indian J. Chem., Sect. B*, 1994, 33, 877, (分離, 誘導體)

Narasimhan, S. et al., Synth. Commun., 1997, 27, 385-390, (合成法)

Nakamura, N. et al., Acta Cryst. C, 1999, 55, 789-791, (結晶構造)

*****ヒノキ (Hinoki) *****

§ § ヒノキ科ヒノキ (*Chamaecyparis obtusa* (Sieb. et Zucc.) Endlicher) の材, 根または枝葉。

§ 8,11,13-Abietatriene-3,12-diol; 3 α -form, 3-Ketone, 1 α ,2 α -epoxy

[化学名・別名] 1 α ,2 α -Epoxy-12-hydroxy-8,11,13-abietatrien-3-one. 1,2-Epoxyhinokione

[化合物分類] テルペノイド (Abietane diterpenoids)

[構造式]

[分子式] $C_{20}H_{26}O_3$

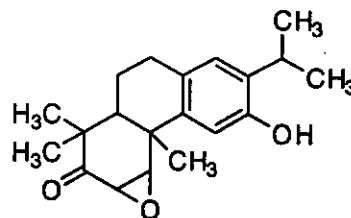
[分子量] 314.424

[基原] *Chamaecyparis obtusa*

[性状] 針状結晶 (Et₂O/hexane)

[融点] Mp 157-159 °C

[比旋光度]: $[\alpha]_D^{24} +224$ (c, 0.66 in CHCl₃)



-----文献-----

Chow, Y.-L. et al., Acta Chem. Scand., 1962, 16, 1296, (分離)

Erdtman, H. et al., Acta Chem. Scand., 1962, 16, 1301, (構造決定)

Lin, Y.-T. et al., J. Chin. Chem. Soc. (Taipei), 1963, 10, 163, (分離)

Ozaki, N. et al., Phytochemistry, 1983, 22, 1771, (分離)

Kutney, J.P. et al., Can. J. Chem., 1992, 70, 1455, (分離, H-NMR, C13-NMR)

Su, W.-C. et al., Phytochemistry, 1994, 35, 1279, (分離, C13-NMR)

§ 3,4:3',4'-Bis(methylenedioxy)lignan-9,9'-olide; (8*R*,8'*R*)-form

[化学名・別名] Hinokinin. Cubebinolide. Heliobupthalmin lactone

[CAS No.] 26543-89-5

[化合物分類] リグナン化合物 (Saturated dibenzylbutyrolactone lignans)

[構造式]

[分子式] $C_{20}H_{18}O_6$

[分子量] 354.359

[基原] Lignan from *Chamaecyparis obtusa* の木部,

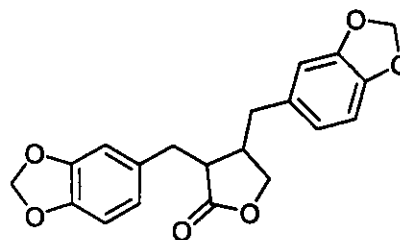
Virola sebifera, その他多くの植物

[性状] 板状結晶 (EtOH or C₆H₆)

[融点] Mp 64-65 °C

[比旋光度]: $[\alpha]_D^{16} -33.7$ (CHCl₃)

UV: [neutral] λ_{max} 235 (ϵ 6760); 287 (ϵ 6760) (MeOH) (Berdy)



-----文献-----

Haworth, R.D. et al., J.C.S., 1938, 1985; 1950, 71, (合成法, 構造決定)

Lopes, L.M.X. et al., Phytochemistry, 1983, 22, 1516, (分離, Mass)

Jakupovic, J. et al., Planta Med., 1986, 18, (分離)

Fang, J.M. et al., Phytochemistry, 1990, 29, 3048, (7'-Oxohinokinin)

Fang, J.M. et al., Phytochemistry, 1992, 31, 3659, (分離)

Lu, X. et al., Synlett, 1993, 68, (合成法, Isohinokinin)

§ 4-Cadinen-10-ol; 10 α -form

[化学名・別名] α -Cadinol

[CAS No.] 481-34-5

[化合物分類] テルペノイド (Cadinane sesquiterpenoids)

[構造式]

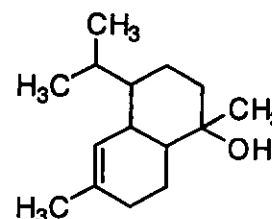
[分子式] $C_{15}H_{26}O$

[分子量] 222.37

[基原] *Chamaecyparis lawsoniana*, *Juniperus communis*. また *Chamaecyparis obtusa*, *Chamaecyparis pisifera*, *Juniperus horizontalis*, *Juniperus scopulorum*, *Athrotaxis* spp., *Neocallitropsis araucaroides*

[性状] 結晶

[融点] Mp 74.5-75 °C



[比旋光度]: $[\alpha]_D^{25} -47$ (-38.5)

文献

Nagasampagi, B.A. et al., Tet. Lett., 1968, 1913, (分離)

Dupreacute, S. et al., Phytochemistry, 1991, 30, 1211, (α -Cadinol methyl ether)

§ Chamaecydin

[CAS No.] 86746-82-9

[化合物分類] テルペノイド (Nor- and homoabietane diterpenoids)

[構造式]

[分子式] $C_{30}H_{40}O_3$

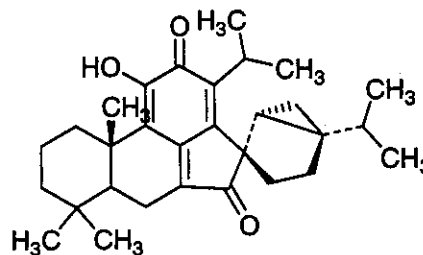
[分子量] 448.644

[基原] *Chamaecyparis obtusa* と *Cryptomeria japonica* の種子

[性状] 黄色のプリズム結晶

[融点] Mp 196-197 °C

[比旋光度]: $[\alpha]_D^{25} +40$ (c, 0.96 in $CHCl_3$)



文献

Hirose, Y. et al., Tet. Lett., 1983, 24, 1535, (分離, 結晶構造)

Shibuya, T., Phytochemistry, 1992, 31, 4289, (分離, H-NMR, C13-NMR)

Su, W.-C. et al., Phytochemistry, 1993, 34, 779, (分離, H-NMR, C13-NMR)

§ Chamaecydin; 22-Epimer

[化学名・別名] Isochamaecydin

[CAS No.] 86699-53-8

[化合物分類] テルペノイド (Nor- and homoabietane diterpenoids)

[構造式]

[分子式] $C_{30}H_{40}O_3$

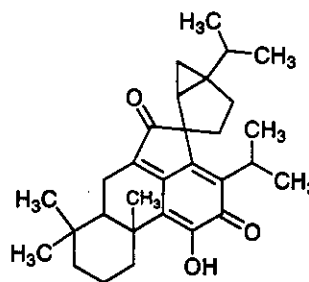
[分子量] 448.644

[基原] *Chamaecyparis obtusa*

[性状] 黄色の針状結晶

[融点] Mp 213-214 °C

[比旋光度]: $[\alpha]_D^{25} +226$ (c, 0.74 in $CHCl_3$)



文献

Hirose, Y. et al., Tet. Lett., 1983, 24, 1535, (分離, 結晶構造)

Shibuya, T., Phytochemistry, 1992, 31, 4289, (分離, H-NMR, C13-NMR)

Su, W.-C. et al., Phytochemistry, 1993, 34, 779, (分離, H-NMR, C13-NMR)

§ Chamaecydin; 6 α -Hydroxy

[化学名・別名] Chamaecydinol. 6 α -Hydroxychamaecydin

[CAS No.] 86699-52-7

[化合物分類] テルペノイド (Nor- and homoabietane diterpenoids)

[構造式]

[分子式] $C_{30}H_{40}O_4$

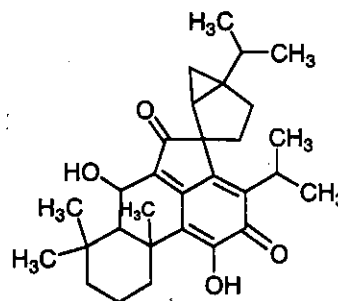
[分子量] 464.644

[基原] *Chamaecyparis obtusa*, *Cryptomeria japonica*

[性状] 黄色のプリズム結晶

[融点] Mp 220-221 °C

[比旋光度]: $[\alpha]_D^{25} -113.8$ (c, 0.91 in $CHCl_3$)



文献

Hirose, Y. et al., Tet. Lett., 1983, 24, 1535, (分離, 結晶構造)

Shibuya, T., Phytochemistry, 1992, 31, 4289, (分離, H-NMR, C13-NMR)

Su, W.-C. et al., Phytochemistry, 1993, 34, 779, (分離, H-NMR, C13-NMR)

§ Chamene

[化学名・別名] 5-Methyl-4-methylene-1-(1-methylethyl)cyclopentene (CAS名).
1-Isopropyl-5-methyl-4-methylenecyclopentene

[CAS No.] 5650-61-3

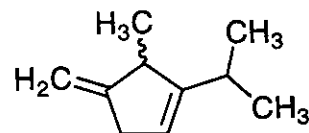
[化合物分類] テルペノイド (Other cyclopentane monoterpenoids)

[構造式]

[分子式] $C_{10}H_{16}$

[分子量] 136.236

[基原] 次の植物のオイルから分離: *Chamaecyparis obtusa*, *Chamaecyparis*



formosensis

[性状] オイル

[沸点] Bp 168-170 °C. Bp₅₀ 86-88 °C

[比旋光度]: $[\alpha]_D +35$

[屈折率] n_D^{20} 1.4686

----- 文献 -----

Kafuku, K. et al., Bull. Chem. Soc. Jpn., 1931, 6, 40; 111, (分離, 構造決定)

Katsura, S., Nippon Kagaku Kaishi, 1942, 63, 1460; CA, 41, 3449a, (分離)

§ 4-Cubebanol; (4 β , 5 β , 6 β , 10 β H)-form

[化学名・別名] 10-Epicubebol

[CAS No.] 176589-53-0

[化合物分類] テルペノイド (Cubebane sesquiterpenoids)

[構造式]

[分子式] $C_{15}H_{26}O$

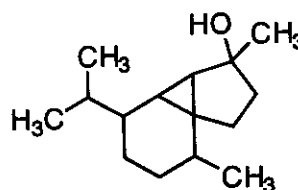
[分子量] 222.37

[基原] *Chamaecyparis obtusa*

[性状] 結晶

[融点] Mp 100 °C

[比旋光度]: $[\alpha]_D -72.3$ (c, 3.3 in $CHCl_3$)



----- 文献 -----

De Rosa, S. et al., Phytochemistry, 1994, 37, 1327-1330, (4-Epicubebol, Cubebol, C13-NMR)

Hieda, T. et al., Phytochemistry, 1996, 42, 159-162, (10-Epicubebol)

§ 4,5-Dihydro-4-(3,4-methylenedioxybenzyl)-3-(3,4-methylenedioxybenzylidene)-2(3H)-furanone; (R,E)-form

[化学名・別名] Savinin. Hibalactone. Taiwanin B

[CAS No.] 493-95-8

[化合物分類] リグナン化合物 (Unsaturated dibenzylbutyrolactone lignans)

[構造式]

[分子式] $C_{20}H_{16}O_6$

[分子量] 352.343

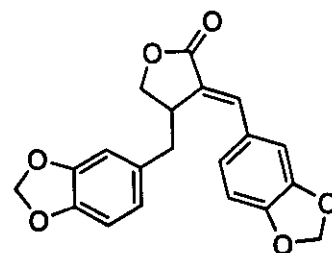
[基原] *Juniperus sabina* と *Juniperus conferta* の針状結晶, *Chloroxylon*

swietenia の樹皮. また *Taiwania cryptomerioides* の心材と *Chamaecyparis obtusa* にも存在する

[性状] 結晶 (C_6H_6 or EtOH)

[融点] Mp 146-148 °C

[比旋光度]: $[\alpha]_D^{21} -87$ (c, 0.95 in $CHCl_3$)



----- 文献 -----

Doi, K. et al., Phytochemistry, 1972, 11, 1175, (分離)

Bhide, K.S. et al., Indian J. Chem., Sect. B, 1977, 15, 440, (分離)

Banerji, J. et al., Phytochemistry, 1984, 23, 2323, (分離)

Shieh, H.-L. et al., J.O.C., 1990, 55, 5139, (結晶構造, conformn)

Fang, J.-M. et al., Phytochemistry, 1992, 31, 3659, (Isohibalactone)

Das, B. et al., Planta Med., 1996, 62, 90, (Isogadain)

§ 11,14-Dihydroxy-8,11,13-abietatrien-7-one

[CAS No.] 209860-29-7

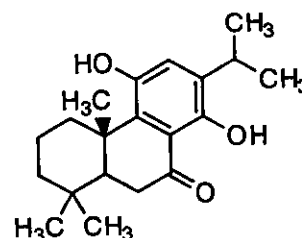
[化合物分類] テルペノイド (Abietane diterpenoids)

[構造式]

[分子式] $C_{20}H_{28}O_3$

[分子量] 316.439

[基原] *Chamaecyparis obtusa* var. *formosana*



[性状] Light 黄色の針状結晶
[融点] Mp 178-179 °C
[比旋光度]: $[\alpha]_D^{24} +65.8$ (c, 0.37 in CHCl₃)
UV: [neutral] λ_{max} 231 (log ϵ 3.94); 273 (log ϵ 3.8) (MeOH)

-----文献-----

Kuo, Y.-H. et al., J. Nat. Prod., 1998, 61, 829-831, (分離, H-NMR, C13-NMR)

§ 4,4'-Dihydroxychalcone

[化学名・別名] 1,3-Bis(4-hydroxyphenyl)-2-propen-1-one
[CAS No.] 3600-61-1
[関連 CAS No.] 108997-30-4
[化合物分類] フラボノイド (Chalcone flavonoids; 2 × O-置換基)

[構造式]

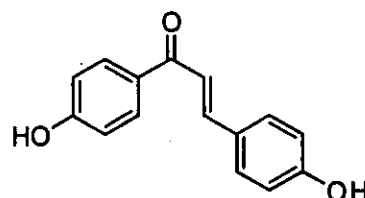
[分子式] C₁₅H₁₂O₃

[分子量] 240.258

[基原] *Chamaecyparis obtusa*

[性状] 黄色の針状結晶 (MeOH 溶液)

[融点] Mp 207-208 °C



-----文献-----

Geissman, T.A. et al., J.A.C.S., 1946, 68, 697, (合成法)
Ohashi, H. et al., Phytochemistry, 1988, 27, 3993, (分離)
Gao, C. et al., Synth. Commun., 1995, 25, 1877, (H-NMR)

§ 3,7-Dimethyl-6-octenoic acid; (S)-form

[CAS No.] 2111-53-7

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

[構造式]

[分子式] C₁₀H₁₈O₂

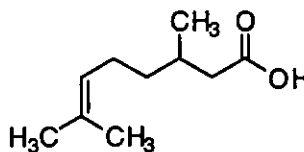
[分子量] 170.251

[基原] *Callitris glauca*, *Callitris intratropica*, *Chamaecyparis obtusa*, *Thujaopsis dolabrata*, *Juniperus* spp., その他の植物

[沸点] Bp_{0.6} 118 °C

[比旋光度]: $[\alpha]_D^{24} -6.6$

[販売元] Aldrich:36442-8; Sigma:C6955



-----文献-----

Lukeys, R. et al., Croat. Chem. Acta, 1957, 29, 201; CA, 53, 17898e, (合成法, 絶対構造)
Valentine, D.V. et al., J.O.C., 1976, 41, 62, (成書)
Opdyke, D.L.J. et al., Food Chem. Toxicol., 1983, 20, 653, (レビュー, 毒性)
He, W. et al., Helv. Chim. Acta, 1995, 78, 391, (合成法)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, CMT125; CMU000

§ Dodecanedioic acid (CAS 名)

[化学名・別名] Decane-1,10-dicarboxylic acid

[CAS No.] 693-23-2

[化合物分類] 脂肪族化合物 (Saturated unbranched carboxylic acids and lactones)

[構造式] HOOC(CH₂)₁₀COOH

[分子式] C₁₂H₂₂O₄

[分子量] 230.303

[基原] 次の植物から分離: *Chamaecyparis obtusa* の葉より得られるワックス

[用途] Monomer for the manuf. of polyesters and polyamides, esp. Nylon-6, 12

[性状] 結晶 (EtOAc)

[融点] Mp 129 °C

[沸点] Bp₁₀ 245 °C

[溶解性] 温水に難溶

[PKa 値] pK_{a1} 5.69; pK_{a2} 6.6 (25 °C, 40% EtOH 溶液)

[販売元] Aldrich:D100-9; Fluka:44050; Sigma:D9630

-----文献-----

- Kariyone, T. et al., Yakugaku Zasshi, 1959, 79, 54, (分離)
 Holmes, J.L. et al., Org. Mass Spectrom., 1970, 3, 1505, (Mass)
 Marosi, L. et al., Annalen, 1973, 584, (性質, 結晶構造)
 Vanier, M. et al., Acta Cryst. B, 1982, 38, 643, (結晶構造)
 Encyclopaedia of Polymer Science and Engineering, Wiley-Interscience, New York, 2nd edn., 1987, 11, 437; 450, (レビュー, polymers)

§ 1,12-Dodecanediol

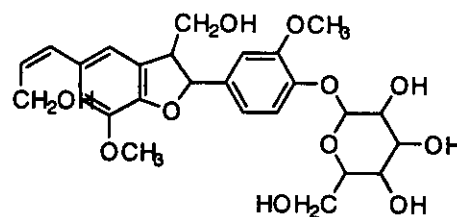
- [化学名・別名] Dodecamethylenediol
 [CAS No.] 5675-51-4
 [化合物分類] 脂肪族化合物 (Saturated unbranched alcohols)
 [構造式] HOCH₂(CH₂)₁₀CH₂OH
 [分子式] C₁₂H₂₆O₂
 [分子量] 202.336
 [基原] 次の植物の葉より得られるワックス: *Chamaecyparis obtusa*, *Pinus thunbergii*
 [性状] 結晶 (EtOH 溶液, または C₆H₆)
 [融点] Mp 80-81 °C
 [沸点] Bp₁₂ 189 °C
 [販売元] Aldrich: D22130-9; Fluka: 44040

-----文献-----

- Drewes, S.E. et al., J.C.S. Perkin 1, 1974, 2578
 Rosen, M.J. et al., J. Am. Oil Chem. Soc., 1976, 53, 742, (di-Ph ether)
 Rao, P.V.S. et al., Oleagineux, 1991, 46, 501; CA, 116, 252152, (di-Ph ether)
 Nakamura, N. et al., Acta Cryst. C, 1997, 53, 1883-1885, (結晶構造)

§ 4,7'-Epoxy-3,8'-bilign-7-ene-3',4',5,9,9'-pentol; (7'S,8'S)-form, 3',5-Di-Me ether, 4'-O-β

- D-glucopyranoside
 [CAS No.] 96738-84-0
 [化合物分類] リグナン化合物 (Neolignans)
 [構造式]
 [分子式] C₂₆H₃₂O₁₁
 [分子量] 520.532
 [基原] *Chamaecyparis obtusa*, *Citrus* spp., *Fortunella japonica*, *Plagiorhagma dubium*
 [融点] Mp 125 °C

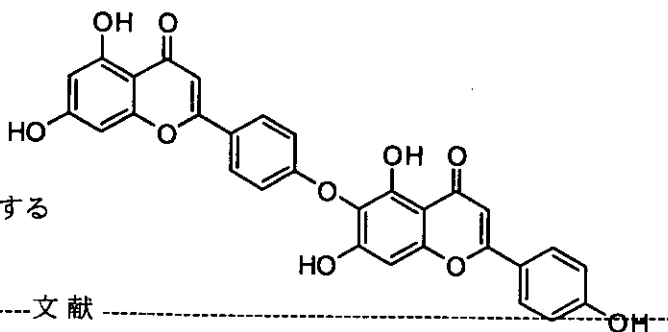


-----文献-----

- Binns, A.N. et al., Proc. Natl. Acad. Sci. U.S.A., 1987, 84, 980, (配糖体)
 Yoshizawa, F. et al., Chem. Pharm. Bull., 1990, 38, 1927, (配糖体)
 Hirai, N. et al., Biosci., Biotechnol., Biochem., 1994, 58, 1679, (絶対構造, 分割)
 Hashimoto, Y. et al., CA, 1994, 121, 251213h

§ Hinokiflavone

- [化学名・別名] 6-[4-(5,7-Dihydroxy-4-oxo-4H-1-benzopyran-2-yl)phenoxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one (CAS名)
 [CAS No.] 19202-36-9
 [化合物分類] フラボノイド (Biflavonoids and polyflavonoids)
 [構造式]
 [分子式] C₃₀H₁₈O₁₀
 [分子量] 538.466
 [基原] *Chamaecyparis obtusa* の葉, また *Psilotum triquetrum* から得られる。
 ヒノキ科, Cycadales, その他多くの植物に存在する
 [性状] 結晶 (hydrate)
 [融点] Mp 353-355 °C で分解

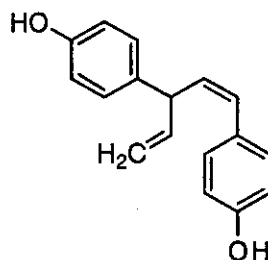


-----文献-----

Voirin, B. et al., C. R. Hebd. Seances Acad. Sci. Ser. D, 1966, 262, 707, (分離)
Miura, H. et al., Chem. Pharm. Bull., 1966, 14, 1404; 1968, 16, 1838, (誘導体)
Gadek, P.A. et al., Phytochemistry, 1982, 21, 889; 1985, 24, 267, (生育)

§ Hinokiresinol; (S)-(E)-form

[化学名・別名] *trans*-Hinokiresinol
[化合物分類] リグナン化合物 (Neolignans)
[構造式]
[分子式] $C_{17}H_{16}O_2$
[分子量] 252.312
[基原] *Chamaecyparis obtusa*
[用途] オエストロゲン作用薬
[比旋光度]: $[\alpha]_D -3$ (c, 1 in Me_2CO)
[その他のデータ] Partial racemate

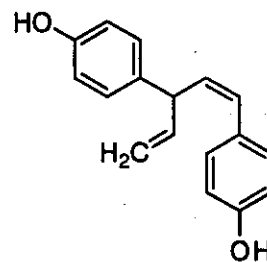


文献

Hirose, Y. et al., Tet. Lett., 1965, 3665, (分離, 構造決定, UV, IR, H-NMR, Mass)
Jeong, S.-J. et al., Planta Med., 1999, 65, 367-368, (4'-O-Methylhinokiresinol)
Minami, E. et al., Chem. Pharm. Bull., 2000, 48, 389-392, (絶対構造, 成書)
Su, B.-N. et al., Phytochemistry, 2000, 53, 1103-1108, (構造決定, 4'-O-Methylhinokiresinol)

§ Hinokiresinol; (S)-(Z)-form

[CAS No.] 96895-25-9
[化合物分類] リグナン化合物 (Norlignans)
[構造式]
[分子式] $C_{17}H_{16}O_2$
[分子量] 252.312
[基原] *Chamaecyparis obtusa* の木部, *Cryptomeria japonica*, *Hypoxis* spp.
[用途] Shows strong oestrogen receptor binding activity
[融点] Mp 102-103 °C

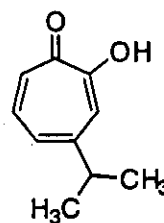


文献

Hirose, Y. et al., Tet. Lett., 1965, 3665, (分離, 構造決定, UV, IR, H-NMR, Mass)
Enzell, C.R. et al., Tet. Lett., 1967, 793; 2211, (絶対構造, Mass)
Jeong, S.-J. et al., Planta Med., 1999, 65, 367-368, (4'-O-Methylhinokiresinol)
Su, B.-N. et al., Phytochemistry, 2000, 53, 1103-1108, (構造決定, 4'-O-Methylhinokiresinol)

§ 2-Hydroxy-4(6)-isopropyl-2,4,6-cycloheptatrien-1-one

[化学名・別名] 2-Hydroxy-4(6)-(1-methylethyl)-2,4,6-cycloheptatrien-1-one (CAS 名). 4(6)-Isopropyltropolone. β -Thujaplicin. Hinokitiol
[CAS No.] 499-44-5
[化合物分類] テルペノイド (Cycloheptane monoterpenoids), 単環芳香族 (Tropolone derivatives)
[構造式]
[分子式] $C_{10}H_{12}O_2$
[分子量] 164.204
[一般的性質] Tautomeric with the 2-oxo-1-hydroxy struct. (equivalent to 6-isopropyl)
[基原] *Juniperus conferta*, *Juniperus chinensis*, *Juniperus communis*, *Juniperus thurifera*, *Juniperus utahensis*, Hinoki tree (*Chamaecyparis obtusa*) の木部のオイル, *Thuja plicata* の心材, *Thuja occidentalis*. ヒノキ科に広く分布する
[用途] 抗カビ物質。また, 強い殺虫作用と植物成長抑制作用を示す
[性状] 結晶 (petrol)
[融点] Mp 52-52.5 °C
[PKa 値] pK_a 6.72 (25 °C, I 2.0)
[傷害・毒性] 50 % 致死量 (LD₅₀) (マウス, 腹膜内) 85 mg/kg
[化学物質毒性データ総覧 (RTECS) 登録番号] GU4200000
[販売元] Aldrich: 46952-1



文献

Anderson, A.B. et al., Acta Chem. Scand., 1948, 2, 644, (分離, 構造決定)
Derry, J.E. et al., J.C.S. Perkin 2, 1972, 694, (結晶構造)

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 573, (生育)

Ohishi, H. et al., Acta Cryst. C, 1994, 50, 587, (結晶構造, 成書)

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, IRR000

RTECS (化学物質毒性データ)

生体影響物質 : 医薬品. 生殖影響物質. 天然物.

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>> 認知されている最低致死量に関する試験

曝露経路 : 経口投与.

被験動物 : げっ歯類-ラット.

投与量・期間 : 500 mg/kg

毒性影響 : [行動] 傾眠(全身活動度の低下).

[行動] 摂餌量(動物).

[胃腸] その他の変化.

参考文献

National Technical Information Service. (Springfield, VA 22161) OTS0570591

生殖に関するデータ

<<試験方法>> 最小毒性量(TDLo).

曝露経路 : 経口投与.

被験動物 : げっ歯類-マウス.

投与 : 560 mg/kg

雌雄投与期間 : 雌 9日間(交配後)

毒性影響 : [生殖] [胚または胎仔に対する影響] 胎仔毒性(死亡をのぞく.たとえば胎仔の发育阻害).

[生殖] [特定の发育異常] 頭骸と顔(鼻と舌を含む).

[生殖] [特定の发育異常] 筋肉骨格系.

参考文献

Food and Chemical Toxicology. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) 37,1097,1999

§ 8(14),15-Isopimaradiene-18,19-diol; 18,19-Isopropylidene

[CAS No.] 209860-30-0

[化合物分類] テルペノイド (Isopimarane diterpenoids)

[構造式]

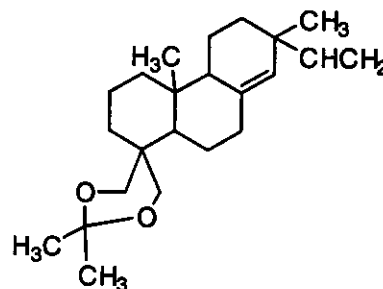
[分子式] $C_{25}H_{36}O_2$

[分子量] 344.536

[基原] *Chamaecyparis obtusa* var. *formosana*

[性状] オイル

[比旋光度]: $[\alpha]_D^{25} -7.1$ (c, 0.13 in $CHCl_3$)



-----文献-----

Kuo, Y.-H. et al., J. Nat. Prod., 1998, 61, 829-831, (分離, H-NMR, C13-NMR)

§ p-Menth-2-en-1-ol

[化学名・別名] 1-Methyl-4-(1-methylethyl)-2-cyclohexen-1-ol (CAS名).

4-Isopropyl-1-methyl-2-cyclohexen-1-ol

[CAS No.] 619-62-5

[関連 CAS No.] 29803-81-4

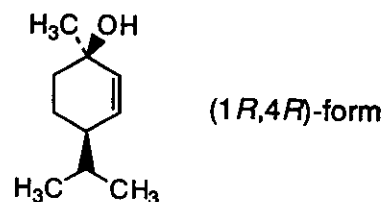
[化合物分類] テルペノイド (p-Menthane monoterpenoids)

[構造式]

[分子式] $C_{10}H_{18}O$

[分子量] 154.252

[基原] *Chamaecyparis obtusa* のオイル



-----文献-----

Naves, Y.R. et al., Bull. Soc. Chim. Fr., 1960, 37, (合成法)

Klein, E. et al., Tetrahedron, 1963, 19, 1091

Schenck, G.O. et al., *Annalen*, 1964, 674, 93
Kuczynski, H. et al., *Pol. J. Chem. (Rocz. Chem.)*, 1966, 40, 643, (合成法)

§ (4-Methyl-1,3-phenylene) biscarbamic acid; Di-Me ester

[化学名・別名] Obtucarbamate A

[CAS No.] 6935-99-5

[構造式]

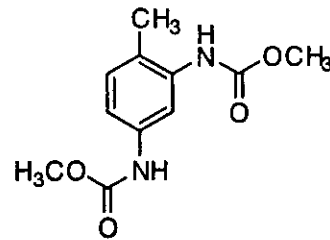
[分子式] $C_{11}H_{14}N_2O_4$

[分子量] 238.243

[基原] *Chamaecyparis obtusa* の樹皮

[性状] 結晶 (MeOH) もしくは針状結晶 (Me₂CO)

[融点] Mp 177 °C (168-169 °C)



----- 文献 -----

Kuo, Y.H. et al., *Chem. Express*, 1990, 5, 909-912, (Obtucarbamate A)

§ 5-Muurolen-4-ol; 4 α-form

[化学名・別名] α-Hinokienol

[CAS No.] 157374-45-3

[化合物分類] テルペノイド (Cadinane sesquiterpenoids)

[構造式]

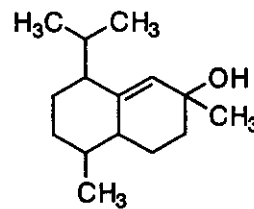
[分子式] $C_{15}H_{26}O$

[分子量] 222.37

[基原] *Cupressus bakeri*, *Chamaecyparis obtusa*

[性状] オイル

[比旋光度]: $[\alpha]_D +80$ (c, 1 in CHCl₃)



----- 文献 -----

Kim, Y.-K. et al., *Phytochemistry*, 1994, 36, 961, (分離, H-NMR, C13-NMR)

Nagashima, F. et al., *Phytochemistry*, 1994, 37, 1323, (分離, H-NMR, C13-NMR)

Hieda, T. et al., *Phytochemistry*, 1996, 42, 159, (Hinokienols)

Cool, L.G. et al., *Phytochemistry*, 1996, 42, 1015, (分離, Mass)

§ 5-Muurolen-4-ol; 4 β-form

[化学名・別名] β-Hinokienol

[CAS No.] 157374-46-4

[化合物分類] テルペノイド (Cadinane sesquiterpenoids)

[構造式]

[分子式] $C_{15}H_{26}O$

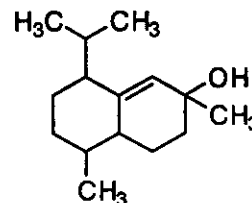
[分子量] 222.37

[基原] *Cupressus bakeri*, *Chamaecyparis obtusa*

[性状] 結晶

[融点] Mp 78 °C

[比旋光度]: $[\alpha]_D +41$ (c, 1 in CHCl₃)



----- 文献 -----

Kim, Y.-K. et al., *Phytochemistry*, 1994, 36, 961, (分離, H-NMR, C13-NMR)

Nagashima, F. et al., *Phytochemistry*, 1994, 37, 1323, (分離, H-NMR, C13-NMR)

Hieda, T. et al., *Phytochemistry*, 1996, 42, 159, (Hinokienols)

Cool, L.G. et al., *Phytochemistry*, 1996, 42, 1015, (分離, Mass)

§ Obtuanhydride

[CAS No.] 209863-21-8

[化合物分類] テルペノイド (Secoabietanes and secofriedoabietane diterpenoids)

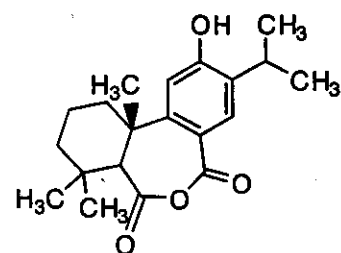
[構造式]

[分子式] $C_{20}H_{26}O_4$

[分子量] 330.423

[基原] *Chamaecyparis obtusa* var. *formosana*

[性状] 黄色の板状結晶



[融点] Mp 167-168 °C

[比旋光度]: $[\alpha]_D^{24} -34$ (c, 0.35 in CHCl₃)

UV: [neutral] λ_{max} 217 (log ϵ 4.08); 233 (log ϵ 4.17); 287 (log ϵ 3.95) (MeOH)

-----文献-----

Kuo, Y.-H. et al., J. Nat. Prod., 1998, 61, 829-831, (分離, H-NMR, C13-NMR)

§ Obtunone

[CAS No.] 203733-43-1

[化合物分類] テルペノイド (Miscellaneous bicyclic diterpenoids)

[構造式]

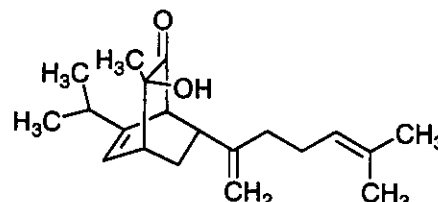
[分子式] C₂₀H₃₀O₂

[分子量] 302.456

[基原] *Chamaecyparis obtusa* var. *formosana*

[性状] オイル

[比旋光度]: $[\alpha]_D^{25} -47.6$ (c, 0.43 in CHCl₃)



-----文献-----

Kuo, Y.-H. et al., Chem. Pharm. Bull., 1998, 46, 181-183, (分離, H-NMR, C13-NMR)

Snider, B.B. et al., Org. Prep. Proced. Int., 1999, 31, 537-541, (合成法, H-NMR, C13-NMR)

§ 3,3',4',5,7-Pentahydroxyflavanone; (2R,3R)-form, 3-O-β

-D-Glucopyranoside

[化学名・別名] Glucodistylin

[CAS No.] 27297-45-6

[化合物分類] フラボノイド (Dihydroflavonols; 5 × O-置換基)

[構造式]

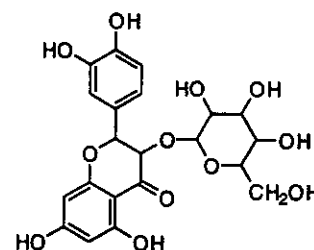
[分子式] C₂₁H₂₂O₁₂

[分子量] 466.398

[基原] *Chamaecyparis obtusa*, *Pinus massoniana*, *Podocarpus* spp., *Aerides fieldingii*, *Zizyphus nummularia*

[融点] Mp 169-171 °C. Mp 325 °C で分解

[比旋光度]: $[\alpha]_D^{20} +36$ (c, 0.2 in MeOH)



-----文献-----

Duebeler, A. et al., Phytochemistry, 1997, 45, 51, (Glucodistylin)

§ 10-Pinanol; (1R,2S,5R)-form, Carboxylic acid

[化学名・別名] 6,6-Dimethylbicyclo[3.3.1]heptane-2-carboxylic acid. 10-Pinanoic acid. Dihydromyrtenic acid

[化合物分類] テルペノイド (Pinane monoterpeneoids)

[構造式]

[分子式] C₁₀H₁₆O₂

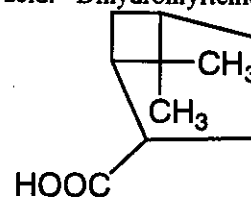
[分子量] 168.235

[基原] 次の植物のオイルから分離: *Chamaecyparis formosensis*, *Chamaecyparis obtusa*

[性状] オイル

[沸点] Bp_s 142-144 °C

[その他のデータ] 立体構造は未決定



-----文献-----

Katsura, S., Nippon Kagaku Kaishi, 1942, 63, 1480, (Dihydromyrtenic acid)

§ 3,11,12-Trihydroxy-8,11,13-abietatrien-7-one; 3 β-form, 3-Ketone, 7 β-alcohol, 12-Me ether

[化学名・別名] 7,11-Dihydroxy-12-methoxy-8,11,13-abietatrien-3-one

[CAS No.] 88143-04-8

[化合物分類] テルペノイド (Abietane diterpenoids)

[構造式]

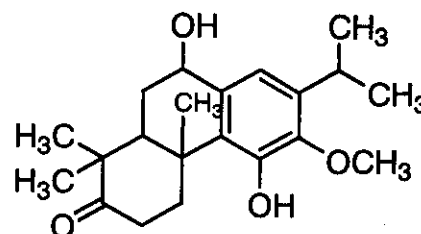
[分子式] C₂₁H₃₀O₄

[分子量] 346.466

[基原] *Chamaecyparis obtusa*

[性状] 針状結晶 (Me₂CO/hexane)

[融点] Mp 224-225 °C



[比旋光度]: $[\alpha]_D^{25} +225$ (c, 0.13 in CHCl₃)
UV: [neutral] λ_{max} 225 (sh); 284 (log ϵ 3.24) (EtOH)

-----文献-----

Ozaki, N. et al., *Phytochemistry*, 1983, 22, 1771-1773, (誘導體)
Kuo, Y.H. et al., *J. Chin. Chem. Soc. (Taipei)*, 1985, 31, 81, (分離)
Yang, S.J. et al., *Phytochemistry*, 1988, 49, 2037-2043, (Taxusabietane A)

*****ヒバ (Hiba) *****

§ § ヒノキ科アスナロ (*Thujopsis dolabrata* Siebold et Zuccarini) の枝葉または材。

§ 8,11,13-Abietatrien-12-ol; 5 α -form, 16-Hydroxy

[化学名・別名] 8,11,13-Abietatriene-12,16-diol. 16-Hydroxyferruginol

[化合物分類] テルペノイド (Abietane diterpenoids)

[構造式]

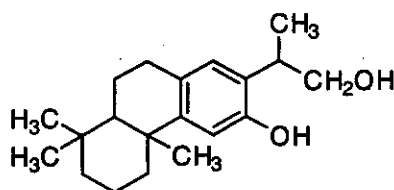
[分子式] C₂₀H₃₀O₂

[分子量] 302.456

[基原] *Thujopsis dolabrata*

[性状] 結晶 (Et:O/pentane)

[比旋光度]: $[\alpha]_D^{29} +36.6$ (c, 0.87 in CHCl₃)



-----文献-----

Matsumoto, T. et al., *Bull. Chem. Soc. Jpn.*, 1991, 64, 2855, (16-Hydroxyferruginol)

Zhao, Q.-S. et al., *Phytochemistry*, 1998, 48, 1025-1029, (16-Hydroxyferruginol, H-NMR, C13-NMR)

§ 15-Beyerene; (-)-form

[CAS No.] 2359-73-1

[化合物分類] テルペノイド (Beyerane diterpenoids)

[構造式]

[分子式] C₂₀H₃₂

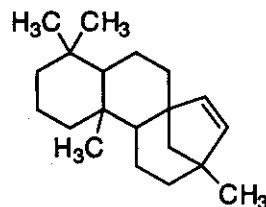
[分子量] 272.473

[基原] 次の植物の精油: *Thujopsis dolabrata*, *Cupressus macrocarpa*, *Podocarpus ferrugineus*

[性状] 結晶もしくはオイル

[融点] Mp 29.5-30 °C

[比旋光度]: $[\alpha]_D^{25} -49.9$ (CHCl₃)



-----文献-----

Kitahara, Y. et al., *Tet. Lett.*, 1964, 1771, (構造決定)

McCrimble, R. et al., *J.C.S. (C)*, 1968, 2349, (分離, 構造決定)

v. Castenn-Lichterfelde, C. et al., *Tetrahedron*, 1977, 33, 1989, (C13-NMR)

Due, D.F.M. et al., *Tetrahedron*, 1978, 34, 1207, (合成法)

§ Cuparene; (R)-form, 15-Hydroxy

[化学名・別名] γ -Cuparenol

[CAS No.] 4584-25-2

[化合物分類] テルペノイド (Cuparane sesquiterpenoids)

[構造式]

[分子式] C₁₅H₂₂O

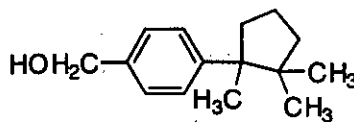
[分子量] 218.338

[基原] *Thujopsis dolabrata*

[性状] オイル

[沸点] Bp_{0.5} 110 °C (bath)

[比旋光度]: $[\alpha]_D^{27} +92$



-----文献-----

Itocirc, S. et al., *Tet. Lett.*, 1965, 3777, (γ -Cuparenol)

§ Deoxydopodophyllic acid

[CAS No.] 38943-33-8

[化合物分類] 薬物: 抗腫瘍薬 (Antineoplastic agents), リグナン化合物 (Side-chain oxygenated aryltetralin lignans)

[構造式]

[分子式] $C_{22}H_{24}O_8$

[分子量] 416.427

[一般的性質] Lignan numbering shown

[基原] 次の植物から分離: *Thujopsis dolabrata*

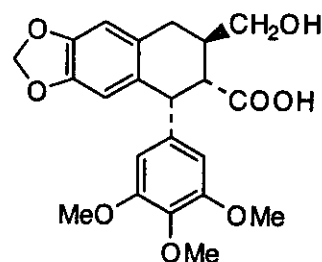
[用途] 抗腫瘍剤

[性状] 結晶 (MeOH)

[融点] Mp 171-172 °C

[比旋光度]: $[\alpha]_D^{25} -158.5$ (Py)

[Log P 計算値] Log P 0.5 (計算値)



----- 文献 -----

Quon, H.H. et al., CA, 1972, 77, 137401, (分離)

Akahori, A. et al., Chem. Pharm. Bull., 1972, 20, 1150, (分離)

Murphy, S.T. et al., Aust. J. Chem., 1975, 28, 81, (分離)

Russell, G.B., Phytochemistry, 1975, 14, 2708, (分離, 誘導体)

§ 3,7-Dimethyl-6-octenoic acid; (S)-form

[CAS No.] 2111-53-7

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

[構造式]

[分子式] $C_{10}H_{18}O_2$

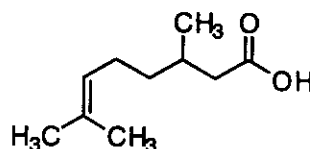
[分子量] 170.251

[基原] *Callitris glauca*, *Callitris intratropica*, *Chamaecyparis obtusa*, *Thujopsis dolabrata*, *Juniperus* spp., その他の植物

[沸点] $Bp_{0.6} 118$ °C

[比旋光度]: $[\alpha]_D^{25} -6.6$

[販売元] Aldrich: 36442-8; Sigma: C6955



----- 文献 -----

Lukešs, R. et al., Croat. Chem. Acta, 1957, 29, 201; CA, 53, 17898e, (合成法, 絶対構造)

Valentine, D.V. et al., J.O.C., 1976, 41, 62, (成書)

Opdyke, D.L.J. et al., Food Chem. Toxicol., 1983, 20, 653, (レビュー, 毒性)

§ β -Dolabrin

[化学名・別名] 2-Hydroxy-4-(1-methylethenyl)-2,4,6-cycloheptatrien-1-one (CAS 名), 4-Isopropenyltropolone

[CAS No.] 4570-11-0

[化合物分類] テルペノイド (Cycloheptane monoterpenoids), 単環芳香族 (Tropolone derivatives)

[構造式]

[分子式] $C_{10}H_{10}O_2$

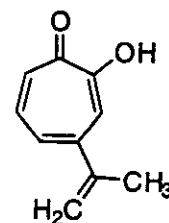
[分子量] 162.188

[基原] *Thujopsis dolabrata* の精油に存在。また *Juniperus* spp., *Cupressus* spp., *Thuja plicata* から得られる

[性状] 青白い黄色の針状結晶

[融点] Mp 58-59 °C

[溶解性] BERDY SOL: ヘキサンに難溶



----- 文献 -----

Nozoe, T. et al., Chem. Ind. (London), 1957, 1070, (分離, UV, 構造決定)

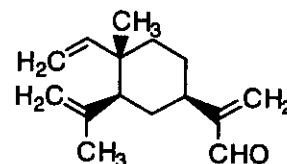
Zavarin, E. et al., J.O.C., 1959, 24, 1318, (分離)

§ 1,3,11(13)-Elematrien-12-al

[化学名・別名] Elemenal

[CAS No.] 4584-28-5

[化合物分類] テルペノイド (Elemene sesquiterpenoids)



[構造式]

[分子式] $C_{15}H_{22}O$

[分子量] 218.338

[基原] *Thujaopsis dolabrata*

[性状] オイル

[比旋光度]: $[\alpha]_D^{60} -11$ ($CHCl_3$)

-----文献-----

Itocirc, S. et al., Tet. Lett., 1965, 3777, (分離)

Maurer, B. et al., Helv. Chim. Acta, 1977, 60, 2177, (分離)

§ 12,16-Epoxy-8,11,13-abietatriene; (15*R*)-form

[CAS No.] 37842-29-8

[化合物分類] テルペノイド (Furanoabietane diterpenoids)

[構造式]

[分子式] $C_{20}H_{28}O$

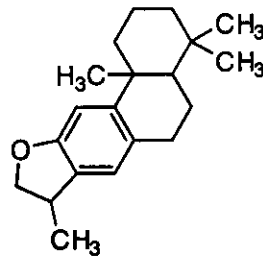
[分子量] 284.441

[基原] *Thujaopsis dolabrata*

[性状] 結晶

[融点] Mp 49-52 °C

[比旋光度]: $[\alpha]_D^{27} +18.9$ (c, 1.06 in $CHCl_3$)



-----文献-----

Hasegawa, S. et al., Phytochemistry, 1982, 21, 643, (分離, 構造決定)

Matsumoto, T. et al., Bull. Chem. Soc. Jpn., 1987, 60, 2401, (合成法, 絶対構造)

§ 4(18),15-Erythroxyadiene; 13 α -form

[化学名・別名] Dolabradiene

[CAS No.] 3650-13-3

[化合物分類] テルペノイド (Erythroxyane diterpenoids)

[構造式]

[分子式] $C_{20}H_{32}$

[分子量] 272.473

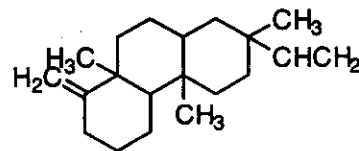
[基原] *Thujaopsis dolabrata*

[性状] オイル

[沸点] Bp₇ 169 °C

[比旋光度]: $[\alpha]_D^{25} -70$ (neat)

[屈折率] $n_D^{20} 1.524$



-----文献-----

Kitahara, Y. et al., Tet. Lett., 1964, 1755; 1763, (分離, IR, H-NMR, 合成法)

Connolly, J.D. et al., Chem. Pharm. Bull., 1965, 13, 603, (構造決定)

Kitadani, M. et al., Chem. Lett., 1974, 963, (構造決定)

§ 4(15),11(13)-Eudesmadien-12-ol; (5 α ,7 β ,10 β)-form, 12-Aldehyde

[化学名・別名] 4(15),11(13)-Eudesmadien-12-al. 4(15),11(13)-Selinadien-12-al. β -Costal

[CAS No.] 3650-40-6

[化合物分類] テルペノイド (Simple eudesmane sesquiterpenoids)

[構造式]

[分子式] $C_{15}H_{22}O$

[分子量] 218.338

[基原] *Thujaopsis dolabrata*, *Chamaecyparis formosensis*

[性状] オイル

[沸点] Bp₁₅ 164-166 °C

[比旋光度]: $[\alpha]_D +24$

[その他のデータ] Originally called α -Costal



-----文献-----

Bawdekar, A.S. et al., Tetrahedron, 1965, 21, 1521; 1967, 23, 1993, (分離, 構造決定)

Maurer, B. et al., Helv. Chim. Acta, 1977, 60, 2177, (分離, H-NMR, IR)