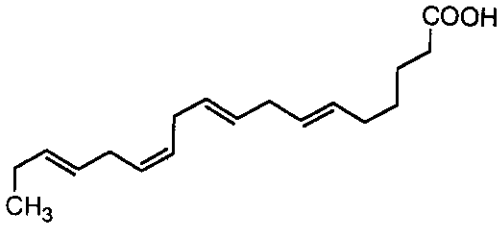
[CAS No.]20290-75-9
[化合物分類]脂肪族化合物(Unbranched alkenic carboxylic acids and lactones)
[構造式]



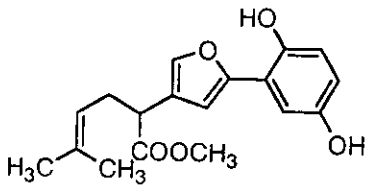
[分子式]$C_{18}H_{28}O_2$
[分子量]276.418
[基原]次の植物から分離: *Lithospermum officinale*, *Onosmodium occidentale*, ニシンとその他の魚のオイル
[性状]青白い黄色のオイル
[融点]Mp 約-57 ℃
[屈折率]n^{16}_D 1.4888

----------文 献----------

Klenk, E. et al., Hoppe Seyler's Z. Physiol. Chem., 1957, 307, 272, (分離)
Craig, B.M. et al., J. Am. Oil Chem. Soc., 1964, 41, 209, (分離)
Griffiths, G. et al., Phytochemistry, 1996, 43, 381, (分離, 生合成)

§§ムラサキ科(*Lithospermum erythrorhizon* Siebold et Zucccarini)の葉または根茎。

§ Deacetylshikonofuran A; 11-Ac
[化学名・別名]Shikonofuran A. Dihydroechinofuran
[CAS No.]85022-66-8
[化合物分類]含酸素複素環式化合物(Furans), 単環芳香族(Simple phenols), テルペノイド(Meroterpenoids)
[構造式]

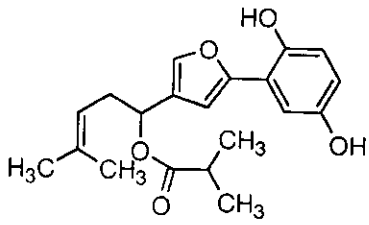


[分子式]$C_{18}H_{20}O_5$
[分子量]316.353
[基原]*Lithospermum erythrorhizon* の根
[性状]結晶 (CH_2Cl_2)
[融点]Mp 74-76 ℃
[比旋光度]:$[\alpha]_D$ -50 (c, 0.52 in $CHCl_3$)

----------文 献----------

Yoshizawa, F. et al., Chem. Pharm. Bull., 1982, 30, 4407, (分離, H-NMR)
Xing-Sheng, Y. et al., Tet. Lett., 1983, 24, 3247
Yazaki, K. et al., Chem. Pharm. Bull., 1986, 34, 2290

§ Deacetylshikonofuran A; 11-*O*-(2-Methylpropanoyl)
[化学名・別名]Shikonofuran D
[CAS No.]85022-63-5
[化合物分類]含酸素複素環式化合物(Furans), 単環芳香族(Simple phenols), テルペノイド(Meroterpenoids)
[構造式]



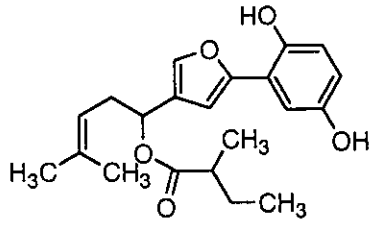
[分子式]$C_{20}H_{24}O_5$
[分子量]344.407
[基原]*Lithospermum erythrorhizon*
[その他のデータ]Shikonofuran E との混合物として分離

----------文 献----------

Yoshizawa, F. et al., Chem. Pharm. Bull., 1982, 30, 4407, (分離, H-NMR)
Xing-Sheng, Y. et al., Tet. Lett., 1983, 24, 3247
Yazaki, K. et al., Chem. Pharm. Bull., 1986, 34, 2290

§ Deacetylshikonofuran A; 11-*O*-(2-Methylbutanoyl)

[化合物分類]テルペノイド(Meroterpenoids), 単環芳香族(Simple phenols), 含酸素複素環式化合物(Furans)
[構造式]

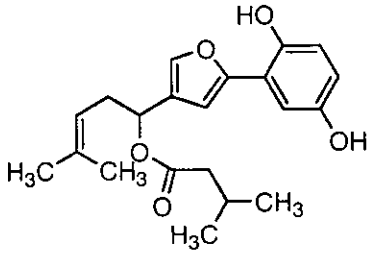


[分子式]$C_{21}H_{26}O_5$
[分子量]358.433
[基原]*Lithospermum erythrorhizon, Arnebia euchroma*
[性状]オイル
[比旋光度]:[α]$_D$ -33.3 (c, 0.48 in $CHCl_3$)

----------文 献 ---------

Yoshizawa, F. et al., Chem. Pharm. Bull., 1982, 30, 4407, (分離, H-NMR)
Xing-Sheng, Y. et al., Tet. Lett., 1983, 24, 3247
Yazaki, K. et al., Chem. Pharm. Bull., 1986, 34, 2290

§ Deacetylshikonofuran A; 11-*O*-(3-Methylbutanoyl)
[化学名・別名]Shikonofuran C
[CAS No.]85022-64-6
[化合物分類]単環芳香族(Simple phenols), 含酸素複素環式化合物(Furans), テルペノイド(Meroterpenoids)
[構造式]

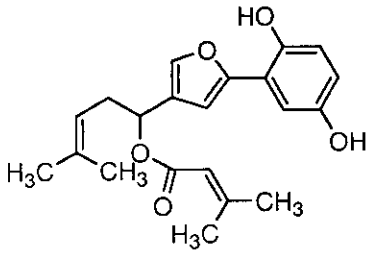


[分子式]$C_{21}H_{26}O_5$
[分子量]358.433
[基原]*Lithospermum erythrorhizon, Arnebia euchroma*
[性状]オイル
[比旋光度]:[α]$_D$ +60 (c, 0.3 in $CHCl_3$)

----------文 献 ----------

Yoshizawa, F. et al., Chem. Pharm. Bull., 1982, 30, 4407, (分離, H-NMR)
Xing-Sheng, Y. et al., Tet. Lett., 1983, 24, 3247
Yazaki, K. et al., Chem. Pharm. Bull., 1986, 34, 2290

§ Deacetylshikonofuran A; 11-*O*-(3-Methyl-2-butenoyl)
[化学名・別名]Shikonofuran E
[CAS No.]85022-62-4
[化合物分類]テルペノイド(Meroterpenoids), 単環芳香族(Simple phenols), 含酸素複素環式化合物(Furans)
[構造式]

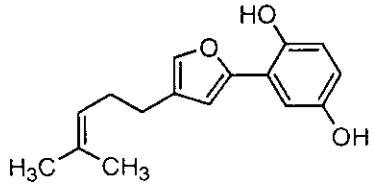


[分子式]$C_{21}H_{24}O_5$
[分子量]356.418
[基原]Intermed. in biosynth. of 5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione in cultured cells of *Litho spermum erythrorhizon*
[性状]オイル
[比旋光度]:[α]$_D$ -68.8 (c, 0.5 in $CHCl_3$)

----------文 献 ----------

Yoshizawa, F. et al., Chem. Pharm. Bull., 1982, 30, 4407, (分離, H-NMR)
Xing-Sheng, Y. et al., Tet. Lett., 1983, 24, 3247
Yazaki, K. et al., Chem. Pharm. Bull., 1986, 34, 2290

§ Deacetylshikonofuran A; 11-Deoxy
[化学名・別名]Deoxyshikonofuran
[化合物分類]含酸素複素環式化合物(Furans), 単環芳香族(Simple phen ols), テルペノイド(Meroterpenoids)
[構造式]



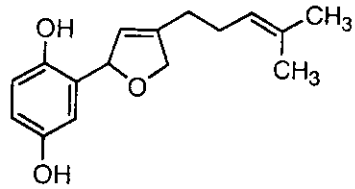
[分子式]$C_{16}H_{18}O_3$
[分子量]258.316

[分子式]$C_{16}H_{18}O_3$
[分子量]258.316
[基原]次の植物から分離: *Lithospermum erythrorhizon* の組織細胞
[用途]5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione 生合成の中間体
[性状]針状結晶
[融点]Mp 139-141 ℃

----------文 献----------

Yoshizawa, F. et al., Chem. Pharm. Bull., 1982, 30, 4407, (分離, H-NMR)
Xing-Sheng, Y. et al., Tet. Lett., 1983, 24, 3247
Yazaki, K. et al., Chem. Pharm. Bull., 1986, 34, 2290

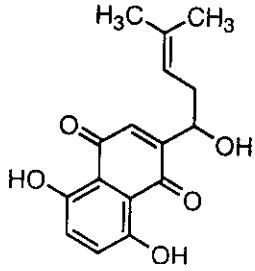
§ Dihydroshikonofuran
[化合物分類]テルペノイド(Meroterpenoids), 単環芳香族(Simple phenols), 含酸素複素環式化合物(Furans)
[構造式]
[分子式]$C_{16}H_{20}O_3$
[分子量]260.332
[基原]*Lithospermum erythrorhizon*
[性状]オイル
[比旋光度]:$[\alpha]_D$ -90.2 (c, 0.4 in $CHCl_3$)



----------文 献----------

Yazaki, K. et al., Chem. Pharm. Bull., 1987, 35, 898, (分離, H-NMR)

§ 5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione; (*R*)-form
[CAS No.]517-89-5
[化合物分類]薬物: 抗菌性剤(Antibacterial agents), 多環芳香族(Naphthoquinones; 2 × O-置換基)
[構造式]
[分子式]$C_{16}H_{16}O_5$
[分子量]288.299
[基原]次の植物から分離: *Lithospermum erythrorhizon*, *Lithospermum officinale*, *Lithospermum euchromum*, *Arnebia nobilis*, *Arnebia tibetana*
[用途]抗菌性剤
[性状]赤-褐色の粉末 (C_6H_6)
[融点]Mp 148 ℃ (143 ℃)
[比旋光度]:$[\alpha]^{20}_{Hg}$ +135 (C_6H_6)
[Log P 計算値]Log P 1.84 (計算値)



UV: [base] λ_{max} (溶媒は報告されていない)(Derep) [neutral] λ_{max} 276 (ε 20000); 488 (ε 1200); 525 (ε 8700); 563 (ε 5900)(MeOH)(Derep)
[その他のデータ]Component of Tokyo violet
[傷害・毒性]50 %致死量(LD_{50})(マウス, 経口) >1000 mg/kg; 50 %致死量(LD_{50})(マウス, 腹膜内) 20 mg/kg
[化学物質毒性データ総覧(RTECS)登録番号]QL8000200

----------文 献----------

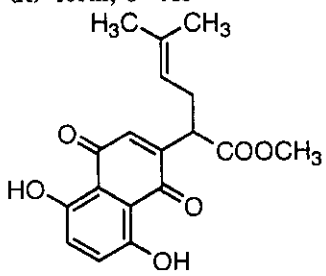
Raudnitz, H. et al., Ber., 1934, 67, 1955; 1935, 68, 1479, (分離, 構造)
Brockmann, H., Annalen, 1935, 521, 1, (分離, 構造)
Arakawa, H. et al., Chem. Ind. (London), 1961, 947, (絶対構造)
Morimoto, I. et al., Tet. Lett., 1965, 3677; 4737; 1966, 3677, (分離, 誘導体)
Shcherbanovskii, L.R. et al., Khim. Prir. Soedin., 1971, 7, 517; Chem. Nat. Compd. (Engl. Transl.), 1971, 7, 491, (分離)
Shukla, Y.N. et al., Phytochemistry, 1971, 10, 1909, (分離, Arnebins)
Schmid, H.V. et al., Tet. Lett., 1971, 4151, (生合成)
Afzal, M. et al., J.C.S. Perkin 1, 1975, 1334, (分離)
Mizukami, H. et al., Phytochemistry, 1978, 17, 95, (分離)
Inouye, H. et al., Phytochemistry, 1979; 18, 1301, (生合成)
Papageorgiou, V.P. et al., Planta Med., 1979, 35, 56, (分離, 構造決定, 用途)
Papageorgiou, V.P. et al., Planta Med., 1979, 37, 259-263; 1980, 39, 81-84, (分離, 誘導体)
Sankawa, U. et al., Chem. Pharm. Bull., 1981, 29, 116, (薬理)

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：20 mg/kg
毒性影響　　：〔行動〕 活動度の変化(特定の試験).
〔行動〕 運動失調.

参照文献
Nippon Yakurigaku Zasshi. Japanese Journal of Pharmacology. 73,193,1977

§ 5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione; (*R*)-form, *O*$^{1'}$-Ac

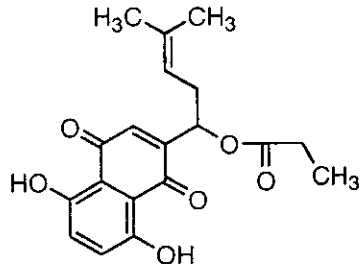


[化学名・別名]Shikonin acetate. Acetylshikonin
[CAS No.]24502-78-1
[化合物分類]多環芳香族(Naphthoquinones; 2 × O-置換基)
[構造式]
[分子式]$C_{18}H_{18}O_6$
[分子量]330.337
[基原]次の植物から分離: *Lithospermum erythrorhizon*, *Lithospermum* *euch* *romum*, *Jatropha glandulifera*
[性状]赤色のプリズム結晶もしくは赤色がかった紫色の針状結晶
[融点]Mp 85-86 ℃. Mp 106-107 ℃

----------文献----------

Fu, S. et al., CA, 1987, 106, 55728f, (Methoxyacetylshikonin)
Papageorgiou, V.P. et al., Angew. Chem., Int. Ed., 1999, 38, 271-300, (レビュー)

§ 5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione; (*R*)-form, *O*$^{1'}$-Propanoyl

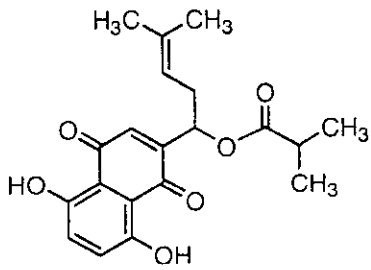


[化学名・別名]Propionylshikonin. Propanoylshikonin
[CAS No.]162283-70-7
[その他の CAS No.]84272-99-1
[化合物分類]多環芳香族(Naphthoquinones; 2 × O-置換基)
[構造式]
[分子式]$C_{19}H_{20}O_6$
[分子量]344.363
[基原]*Lithospermum erythrorhizon*
[用途]抗カビ, 抗ウイルス, 細胞毒性作用を示す

----------文献----------

Li, C. et al., CA, 1998, 128, 241823n, (Propionylshikonin)
Papageorgiou, V.P. et al., Angew. Chem., Int. Ed., 1999, 38, 271-300, (レビュー)

§ 5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione; (*R*)-form, *O*$^{1'}$-(2-Methylpropanoyl)



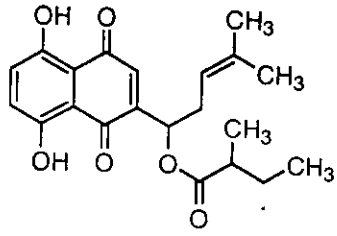
[化学名・別名]Isobutyrylshikonin. Shikonin isobutyrate
[CAS No.]52438-12-7
[化合物分類]多環芳香族(Naphthoquinones; 2 × O-置換基)
[構造式]
[分子式]$C_{20}H_{22}O_6$
[分子量]358.39
[基原]次の植物から分離: *Lithospermum erythrorhizon* の根
[融点]Mp 89-90 ℃
[比旋光度]:$[\alpha]_D^{27}$ 600 +125 (EtOH)

----------文献----------

Brockmann, H., Annalen, 1935, 521, 1, (分離, 構造)
Arakawa, H. et al., Chem. Ind. (London), 1961, 947, (絶対構造)
Morimoto, I. et al., Tet. Lett., 1965, 3677; 4737; 1966, 3677, (分離, 誘導体)
Shcherbanovskii, L.R. et al., Khim. Prir. Soedin., 1971, 7, 517; Chem. Nat. Compd. (Engl. Transl.), 1971, 7, 491, (分離)

Arakawa, H. et al., Chem. Ind. (London), 1961, 947, (絶対構造)
Morimoto, I. et al., Tet. Lett., 1965, 3677; 4737; 1966, 3677, (分離, 誘導体)
Shcherbanovskii, L.R. et al., Khim. Prir. Soedin., 1971, 7, 517; Chem. Nat. Compd. (Engl. Transl.), 1971, 7, 491, (分離)
Li, C. et al., CA, 1998, 128, 241823n, (Propionylshikonin)
Papageorgiou, V.P. et al., Angew. Chem., Int. Ed., 1999, 38, 271-300, (レビュー)

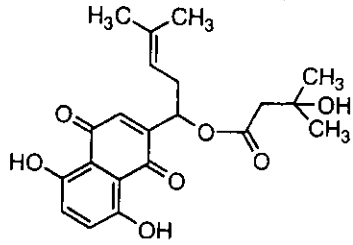
§ 5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl) -1,4-naphthalenedione; (*R*) -form, *O*$^{1'}$-(2-Methylbutanoyl)



[化学名・別名] α-Methylbutyrylshikonin
[CAS No.] 52387-15-2
[化合物分類] 多環芳香族(Naphthoquinones; 2 × O-置換基)
[構造式]
[分子式] $C_{21}H_{24}O_6$
[分子量] 372.417
[基原] *Lithospermum erythrorhizon*, その他の植物属

----------文 献----------
Raudnitz, H. et al., Ber., 1934, 67, 1955; 1935, 68, 1479, (分離, 構造)
Brockmann, H., Annalen, 1935, 521, 1, (分離, 構造)
Arakawa, H. et al., Chem. Ind. (London), 1961, 947, (絶対構造)
Morimoto, I. et al., Tet. Lett., 1965, 3677; 4737; 1966, 3677, (分離, 誘導体)
Shcherbanovskii, L.R. et al., Khim. Prir. Soedin., 1971, 7, 517; Chem. Nat. Compd. (Engl. Transl.), 1971, 7, 491, (分離)
Afzal, M. et al., J.C.S. Perkin 1, 1975, 1334, (分離)
Mizukami, H. et al., Phytochemistry, 1978, 17, 95, (分離)
Inouye, H. et al., Phytochemistry, 1979; 18, 1301, (生合成)
Papageorgiou, V.P. et al., Planta Med., 1979, 35, 56, (分離, 構造決定, 用途)
Salam, N.A. et al., Acta Pharm. Jugosl., 1981, 31, 237-241, (Benzoylshikonin)
Papageorgiou, V.P. et al., Angew. Chem., Int. Ed., 1999, 38, 271-300, (レビュー)

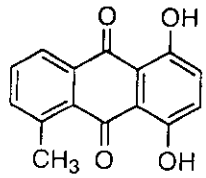
§ 5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl) -1,4-naphthalenedione; (*R*) -form, *O*$^{1'}$-(3-Hydroxy-3-methylbutanoyl)



[化学名・別名] β-Hydroxyisovalerylshikonin
[CAS No.] 7415-78-3
[化合物分類] 多環芳香族(Naphthoquinones; 2 × O-置換基)
[構造式]
[分子式] $C_{21}H_{24}O_7$
[分子量] 388.416
[基原] 次の植物から分離: *Lithospermum erythrorhizon*, *Lithospermum euchromum*
[性状] 赤-紫色の結晶
[融点] Mp 90-92 ℃
[比旋光度]: $[\alpha]_D^{15}$ 600 +128 (EtOH)

----------文 献----------
Terada, A. et al., Chem. Comm., 1983, 987, (合成法)
Khan, H.A. et al., Phytochemistry, 1983, 22, 614-615, (β-Hydroxyisovalerylalkannin)
Papageorgiou, V.P. et al., Angew. Chem., Int. Ed., 1999, 38, 271-300, (レビュー)

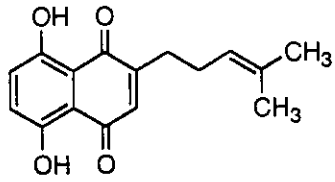
§ 1,4-Dihydroxy-5-methylanthraquinone



[化学名・別名] 5-Methylquinizarin, Skikizarin
[化合物分類] 多環芳香族(9,10-Anthraquinones; 2 × O-置換基)
[構造式]
[分子式] $C_{15}H_{10}O_4$
[分子量] 254.242
[基原] 次の植物から分離: *Lithospermum erythrorhizon* の根
[性状] 赤色の針状結晶 (MeOH)
[融点] Mp 246-247 ℃ (234-235 ℃)

§ 5,8-Dihydroxy-2-(4-methyl-3-pentenyl)-1,4-naphthoquinone

[化学名・別名]5,8-Dihydroxy-2-(4-methyl-3-pentenyl)-1,4-naphthalenedione(CAS 名). Deoxyshikonin. Arnebin VII



[CAS No.]43043-74-9

[化合物分類]多環芳香族(Naphthoquinones; 2 × O-置換基)

[構造式]

[分子式]$C_{16}H_{16}O_4$

[分子量]272.3

[基原]*Alkanna hirsutissima, Arnebia nobilis, Lithospermum erythrorhizon, Macrotomia euchroma, Macrotomia cephatotes, Echium vulgare, Lappula consanguinea, Lappula echinata, Eritrichium incanum, Eritrichium sichotenze, Cynoglossum officinale, Mertensia maritima*

[性状]赤色の針状結晶 (hexane)

[融点]Mp 95 ℃ (92-93 ℃)

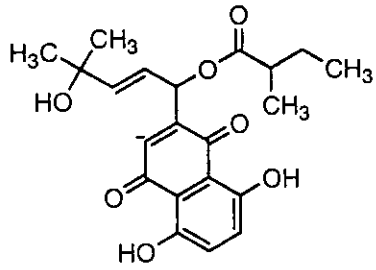
----------文献----------

Dhar, M.M. et al., Indian J. Chem., 1973, 11, 528, (分離, 構造)

Azfal, M. et al., J.C.S. Perkin 1, 1975, 1334, (分離, 構造)

§ 2-(1,4-Dihydroxy-4-methylpentyl)-5,8-dihydroxy-1,4-naphthoquinone; (*R*)-form, 2',3'-Didehydro, 1'-*O*-(2-methylbutanoyl)

[化学名・別名]Lithospermidin A



[CAS No.]83415-78-5

[化合物分類]多環芳香族(Naphthoquinones; 2 × O-置換基)

[構造式]

[分子式]$C_{21}H_{24}O_7$

[分子量]388.416

[基原]*Lithospermum erythrorhizon*

----------文献----------

Hisamichi, S. et al., CA, 1982, 97, 178739p, (Lithospermidins)

§ 2-(1,4-Dihydroxy-4-methylpentyl)-5,8-dihydroxy-1,4-naphthoquinone; (*R*)-form, 2',3'-Didehydro, 1'-*O*-(3-methylbutanoyl)

[化学名・別名]Lithospermidin B

[CAS No.]83415-79-6

[化合物分類]多環芳香族(Naphthoquinones; 2 × O-置換基)

[構造式]構造式は有効ではない

[分子式]$C_{21}H_{24}O_7$

[分子量]388.416

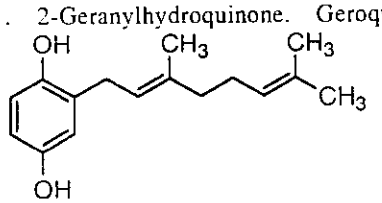
[基原]*Lithospermum erythrorhizon*

----------文献----------

Hisamichi, S. et al., CA, 1982, 97, 178739p, (Lithospermidins)

§ 2-(3,7-Dimethyl-2,6-octadienyl)-1,4-benzenediol

[化学名・別名](3,7-Dimethyl-2,6-octadienyl)hydroquinone(旧 CAS 名). 2-Geranylhydroquinone. Geroquinol, INN. Beradia. B158



[CAS No.]10457-66-6

[関連 CAS No.]80496-91-9

[化合物分類]薬物: 放射線防御剤(Radioprotective agents), テルペノイド(Meroterpenoids), 単環芳香族(Simple phenols)

[構造式]

[分子式]$C_{16}H_{22}O_2$

[分子量]246.349

[一般的性質]For higher homologues see Farnesylhydroquinone and 2-Polyprenyl-1,4-benzenediol

[基原]次の植物から分離: trichomes of *Phacelia ixodes*. また *Lithospermum erythrorhizon* の組織細胞から得られる

[用途]放射線防御剤. 5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione 生合成の中間体

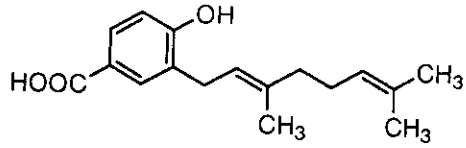
[性状]オイル

[一般的性質]For higher homologues see Farnesylhydroquinone and 2-Polyprenyl-1,4-benzenediol
[基原]次の植物から分離: trichomes of *Phacelia ixodes*. また *Lithospermum erythrorhizon* の組織細胞から得られる
[用途]放射線防御剤. 5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione 生合成の中間体
[性状]オイル
[Log P 計算値]Log P 4.84 (計算値)
[傷害・毒性]接触アレルゲン

----------文 献----------

Fr. Pat., 1964, M2694; CA. 1964, 61, 15940e, (合成法, 薬理, 毒性)
Rudali, G., C. R. Hebd. Seances Soc. Biol. Ses Fil., 1966, 160, 1365, (薬理)
Sato, A. et al., J. Nat. Prod., 1989, 52, 975, (誘導体)
Rueda, A. et al., Nat. Prod. Lett., 1998, 11, 127; 130, (誘導体)

§ 3-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxybenzoic acid; (*E*)-form
[化学名・別名]3-Geranyl-4-hydroxybenzoic acid
[CAS No.]68631-48-1
[化合物分類]テルペノイド(Meroterpenoids), 単環芳香族(Simple benzoic acids and esters)
[構造式]

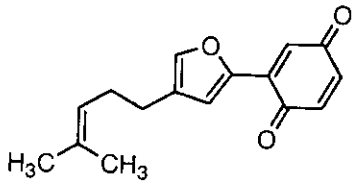


[分子式]$C_{17}H_{22}O_3$
[分子量]274.359
[基原]次の植物から分離: *Lithospermum erythrorhizon* の組織細胞. *Piper murrayanum* の葉
[用途]5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione 生合成の中間体
[性状]板状結晶 (hexane/Me_2CO)
[融点]Mp 74-76 ℃ (67-69 ℃)
[その他のデータ]またオイルとして記載されている

----------文 献----------

Cristina, D. et al., Phytochemistry, 1999, 51, 899-902, (3-Geranyl-4-methoxybenzoic acid)

§ Echinofuran; Deacetoxy
[化学名・別名]Echinofuran B
[CAS No.]90685-55-5
[化合物分類]単環芳香族(Benzoquinones; no O-置換基), 含酸素複素環式化合物(Furans)
[構造式]

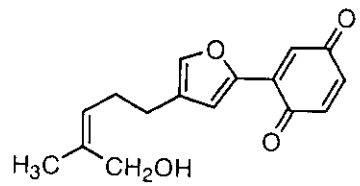


[分子式]$C_{16}H_{16}O_3$
[分子量]256.301
[基原]*Lithospermum erythrorhizon* のカルス培養
[性状]橙色のオイル

----------文 献----------

Fukui, H. et al., Phytochemistry, 1984, 23, 301; 1998, 47, 1037-1039, (Echinofuran B, 6''-Hydroxyechinofuran B)

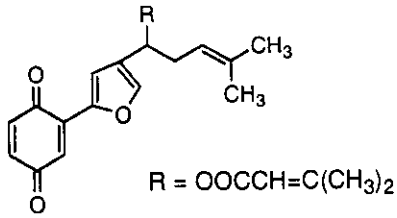
§ Echinofuran; 6''-Hydroxy, deacetoxy
[化学名・別名]6''-Hydroxyechinofuran B
[化合物分類]含酸素複素環式化合物(Furans), 単環芳香族(Benzoquinones; no O-置換基)
[構造式]



[分子式]$C_{16}H_{16}O_4$
[分子量]272.3
[基原]*Lithospermum erythrorhizon*
[性状]褐色のオイル
UV: [neutral] λ_{max} 260 (log ε 4.13); 465 (log ε 3.55) ($CHCl_3$)

----------文 献----------

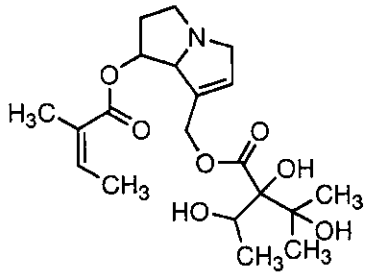
Inouye, H. et al., Phytochemistry, 1981, 20, 1701, (Echinofuran)
Fukui, H. et al., Phytochemistry, 1984, 23, 301; 1998, 47, 1037-1039, (Echinofuran B, 6''-Hydroxyechinofuran B)

[構造式]


[分子式] $C_{21}H_{22}O_5$
[分子量] 354.402
[基原] 次の植物から分離: *Lithospermum erythrorhizon* の根とカルス培養
[性状] 橙-黄色の針状結晶
[融点] Mp 72-74 ℃
[比旋光度]: $[\alpha]_D^{20}$ -81

----------文献----------

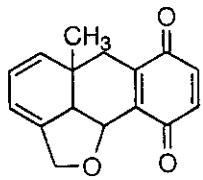
Fukui, H. et al., Phytochemistry, 1984, 23, 301, (分離)

§ Echiumine; 2''*E*-Isomer, 1'''-hydroxy
[化学名・別名] Hydroxymyoscorpine
[CAS No.] 126642-92-0
[化合物分類] アルカロイド化合物 (Simple pyrrolizidine alkaloids)
[構造式]


[分子式] $C_{20}H_{31}NO_7$
[分子量] 397.467
[基原] 次の植物から得られるアルカロイド: *Lithospermum erythrorhizon* の根 (ムラサキ科)
[比旋光度]: $[\alpha]_D$ +2.2 (c, 0.2 in EtOH)

----------文献----------

Roeder, E. et al., Phytochemistry, 1990, 29, 690; 1991, 30, 3107, (Hydroxymyoscorpine, Myoscorpine *N*-oxide)

§ Rhizonone
[CAS No.] 240811-82-9
[化合物分類] テルペノイド (Meroterpenoids), 多環芳香族 (1,2- and 1,4-Anthraquinones), 多環芳香族 (Furoanthracenes)
[構造式]


[分子式] $C_{16}H_{14}O_3$
[分子量] 254.285
[基原] 次の植物から分離: *Lithospermum erythrorhizon* の毛状根の培養物
[性状] オイル
[比旋光度]: $[\alpha]_D$ -240 (c, 0.025 in MeOH), $[\alpha]_D^{437}$ +700 (c, 0.025 in MeOH)
UV: [neutral] λ_{max} 254 (log ε 4.29) ($CHCl_3$)

----------文献----------

Fukui, H. et al., Phytochemistry, 1999, 51, 511-515, (分離, UV, IR, H-NMR, C13-NMR, Mass)

***********メスキート (Mesquite) ***********

§§ マメ科 (*Prosopis juliflora* de Candlle) の材または樹皮。

§ *Prosopis juliflora* Compound C
[化合物分類] 構造未知の天然物
[分子式] $C_{36}H_{60}O_8$
[分子量] 620.865
[一般的性質] 構造は未知
[基原] 次の植物から分離: *Prosopis juliflora* の茎皮
[性状] プリズム結晶 ($CHCl_3/C_6H_6$)
[融点] Mp 185 ℃

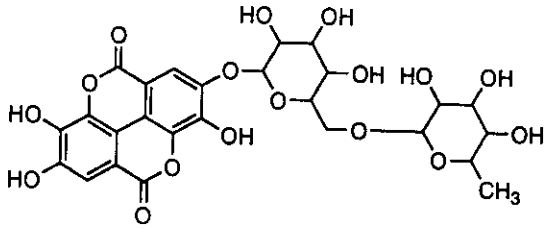
----------文献----------

Vajpeyi, R. et al., Indian J. Chem., Sect. B, 1981, 20, 348, (分離, 性質)

§ Ellagic acid; 2-*O*-[α-L-Rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside]

Vajpeyi, R. et al., Indian J. Chem., Sect. B, 1981, 20, 348, (分離, 性質)

§ **Ellagic acid; 2-*O*-[α-L-Rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside]**
[化学名・別名]Ellagic acid 4-rutinoside
[CAS No.]81099-68-5
[化合物分類]タンニン化合物(Hexahydroxydiphenoyl ester tannins)
[構造式]

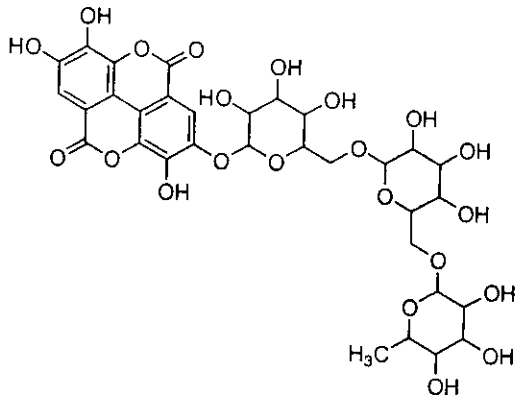


[分子式]$C_{26}H_{28}O_{17}$
[分子量]610.481
[基原]次の植物から分離: *Prosopis juliflora* のさや
[性状]淡い橙-ピンク色の結晶 (Me_2CO/Et_2O)
[融点]Mp 253 ℃で分解
[比旋光度]:$[\alpha]_D^{25}$ -41 (Py)

----------文 献----------

Arthur, H.R., Aust. J. Chem., 1969, 22, 597-600, (分離)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1143, (生育)
Malhotra, S. et al., Phytochemistry, 1981, 20, 860-861; 2043-2044; 2439-2440, (2-rhamnosylglucosylglucosyl, 3,8-di-Me ether 2-rhamnoside, 2-rhamnosylglucosyl)
Yoshida, T. et al., Chem. Pharm. Bull., 1994, 42, 1803-1807, (2-glucoside)

§ **Ellagic acid; 2-*O*-[α-L-Rhamnopyranosyl-(1 → 6)-β-D-glucopyranosyl-(1 → 6)-β-D-glucopyranoside]**
[CAS No.]79284-68-7
[化合物分類]タンニン化合物(Hexahydroxydiphenoyl ester tannins)
[構造式]

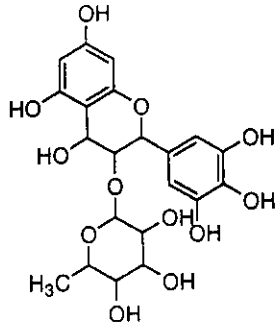


[分子式]$C_{32}H_{38}O_{22}$
[分子量]772.623
[基原]次の植物から分離: *Prosopis juliflora* のさや
[性状]淡黄色のプリズム結晶(Me_2CO/Et_2O)
[融点]Mp 243-245 ℃

----------文 献----------

Okuda, T., Chem. Pharm. Bull., 1961, 9, 178-181, (分離, 誘導体)
Briggs, L.H. et al., J.C.S., 1961, 642-645, (2,3,8-tri-Me ether, 分離)
Row, L.R., Tetrahedron, 1962, 18, 357-360, (2,8-di-Me glucoside, 分離)
Mathieson, A.M. et al., Acta Cryst. B, 1968, 24, 1456-1461, (結晶構造)
Arthur, H.R., Aust. J. Chem., 1969, 22, 597-600, (分離)
Press, R.E. et al., J. Appl. Chem., 1969, 19, 247, (性質)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1143, (生育)
Lin, L.-Z. et al., Huaxue Xuebao, 1979, 37, 207-214; CA, 92, 99499d, (分離, methylene derivs)
Malhotra, S. et al., Phytochemistry, 1981, 20, 860-861; 2043-2044; 2439-2440, (2-rhamnosylglucosylglucosyl, 3,8-di-Me ether 2-rhamnoside, 2-rhamnosylglucosyl)
Yoshida, T. et al., Chem. Pharm. Bull., 1994, 42, 1803-1807, (2-glucoside)
Kim, J.-P. et al., Phytochemistry, 2001, 57, 587-591, (3-Me 8-rhamnoside)

§ **3,3',4,4',5,5',7-Heptahydroxyflavan; 3-*O*-α-L-Rhamnopyranoside**
[化学名・別名]Leucodelphinidin 3-rhamnoside
[CAS No.]76532-04-2
[化合物分類]フラボノイド(Leucoanthocyanidins)
[構造式]



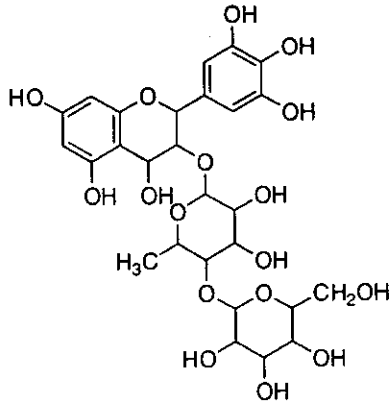
[分子式] $C_{21}H_{24}O_{12}$
[分子量] 468.413
[基原] 次の植物から分離: *Acacia leucophloea* の茎皮, *Prosopis juliflora*

----------文献----------

Ganguly, A.K. et al., Tetrahedron, 1958, 3, 225, (分離)
Murthy, V.K. et al., Tetrahedron, 1965, 21, 1445, (分離)
Trivedi, K.K. et al., Curr. Sci., 1984, 53, 367, (3-rhamnoside)
Onda, M. et al., J. Nat. Prod., 1989, 52, 1100, (分離, 合成法)

§ 3,3',4,4',5,5',7-Heptahydroxyflavan; 3-*O*-[β-D-Glucopyranosyl-(1 → 4)-α-L-rhamnopyranoside]

[CAS No.] 76520-51-9
[化合物分類] フラボノイド (Leucoanthocyanidins)
[構造式]



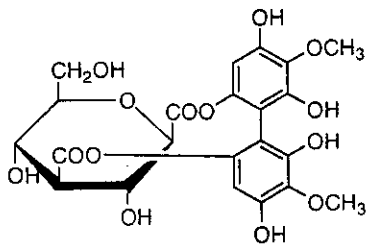
[分子式] $C_{27}H_{34}O_{17}$
[分子量] 630.555
[基原] 次の植物から分離: *Prosopis juliflora* の樹皮とさや

----------文献----------

Ganguly, A.K. et al., Tetrahedron, 1958, 3, 225, (分離)
Murthy, V.K. et al., Tetrahedron, 1965, 21, 1445, (分離)
Malhotra, S. et al., Indian J. Chem., Sect. B, 1983, 22, 936, (3-glucosylrhamnoside)

§ 1,3-Hexahydroxydiphenoylglucose; β-D-Pyranose-form, 4',4''-Di-Me ether

[CAS No.] 87042-28-2
[化合物分類] タンニン化合物 (Hexahydroxydiphenoyl ester tannins)
[構造式]



[分子式] $C_{22}H_{22}O_{14}$
[分子量] 510.407
[基原] 次の植物から分離: *Prosopis juliflora* の根

----------文献----------

Malhotra, S. et al., Curr. Sci., 1983, 52, 583, (分離)
Sheichenko, O.P. et al., Khim. Prir. Soedin., 1987, 902, (Hiporhamnin)

§ 26-Hydroxy-2-hexacosanone (CAS 名)

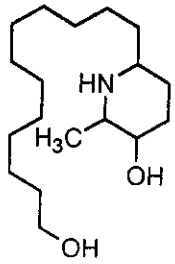
[CAS No.] 78182-87-3
[化合物分類] 脂肪族化合物 (Saturated unbranched aldehydes and ketones)
[構造式] $H_3CCO(CH_2)_{23}CH_2OH$
[分子式] $C_{26}H_{52}O_2$
[分子量] 396.696
[基原] 次の植物から分離: *Prosopis juliflora* の茎皮
[性状] 針状結晶 (Me_2O/hexane)

[性状]針状結晶 (Me$_2$O/hexane)
[融点]Mp 65 ℃

----------文 献----------

Vajpeyi, R. et al., Indian J. Chem., Sect. B, 1981, 20, 348, (分離, 構造)

§ Julifloridine; (2*R,5*R**,6*R**)-form**

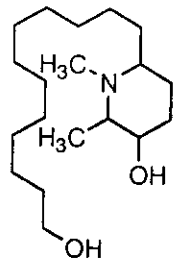


[CAS No.]66731-40-6
[化合物分類]アルカロイド化合物(Simple piperidine alkaloids)
[構造式]
[分子式]$C_{18}H_{37}NO_2$
[分子量]299.496
[基原]次の植物のアルカロイド微量成分: *Prosopis juliflora* の葉 (マメ科)
[融点]Mp 82-83 ℃
[比旋光度]:[α]$_D$ +18 (c, 0.84 in MeOH) (synthetic)

----------文 献----------

Ahmad, V.U. et al., Z. Naturforsch., B, 1978, 33, 347, (分離, Mass, 構造)
Ahmad, V.U. et al., Sci. Pharm., 1990, 58, 409, (*N*-Methyljulifloridine)
Kiguchi, T. et al., Tetrahedron, 1998, 54, 15589-15606, (合成法, 構造)
Astudillo, S.L. et al., Planta Med., 1999, 65, 161-162, (分離, H-NMR, C13-NMR, Mass)

§ Julifloridine; (±)-form, *N*-Me

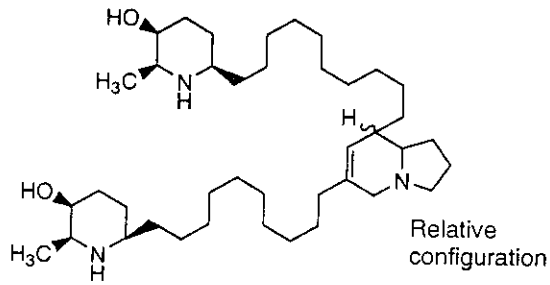


[化学名・別名]5-Hydroxy-1,6-dimethyl-2-piperidinedodecanol. *N*-Methyljulifloridine
[CAS No.]132972-82-8
[化合物分類]アルカロイド化合物(Simple piperidine alkaloids)
[構造式]
[分子式]$C_{19}H_{39}NO_2$
[分子量]313.523
[基原]次の植物から得られるアルカロイド: *Prosopis juliflora* (マメ科)
[その他のデータ]Struct. requires revision (1998)

----------文 献----------

Ahmad, V.U. et al., Z. Naturforsch., B, 1978, 33, 347, (分離, Mass, 構造)
Ahmad, V.U. et al., Sci. Pharm., 1990, 58, 409, (*N*-Methyljulifloridine)
Astudillo, S.L. et al., Planta Med., 1999, 65, 161-162, (分離, H-NMR, C13-NMR, Mass)

§ Juliflorine



[化学名・別名]Juliprosopine
[CAS No.]76202-00-1
[化合物分類]アルカロイド化合物(Indolizidine alkaloids), アルカロイド化合物(Miscellaneous piperidine alkaloids), アルカロイド化合物(Simple piperidine alkaloids)
[構造式]
[分子式]$C_{40}H_{75}N_3O_2$
[分子量]630.051
[一般的性質]The two piperidine systems need not have the same abs. config.
[基原]次の植物から得られるアルカロイド: *Prosopis juliflora* (マメ科)
[用途]抗菌性と抗カビ作用を示す
[性状]非結晶性
[比旋光度]:[α]$_D$ +0.7 (c, 1.05 in EtOH), [α]$_D$ +10 (c, 2.15 in $CHCl_3$)
[溶解性]BERDY SOL: メタノール, クロロホルムに可溶; 水に難溶
[その他のデータ]いくつかの *O*, *N*-acetyl と *N*-Me 誘導体は非結晶性
[化学物質毒性データ総覧(RTECS)登録番号]TN7637000

----------文 献----------

Ahmad, V.U. et al., Z. Naturforsch., B, 1978, 33, 347, (分離)
Aqeel, A. et al., Arzneim.-Forsch., 1989, 39, 652, (性質, Julifloricine)
Ahmad, V.U. et al., J. Nat. Prod., 1989, 52, 497, (Juliflorinine)

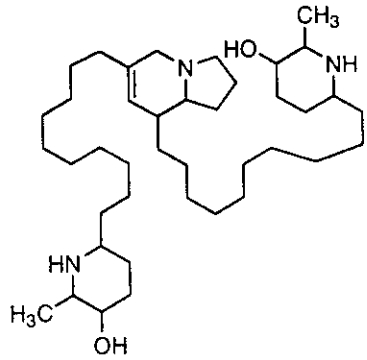
***RTECS (化学物質毒性データ) ***

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　　：腹腔内投与.
被験動物　　：げっ歯類-マウス.
投与量・期間：17460 ug/kg
毒性影響　　：〔行動〕傾眠(全身活動度の低下).

参照文献
Arzneimittel-Forschung. Drug Research.(Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) 41,151,1991

§ Juliflorine; Stereoisomer
[化学名・別名]Julifloricine
[CAS No.]66771-80-0
[化合物分類]アルカロイド化合物(Indolizidine alkaloids), アルカロイド化合物(Miscellaneous piperidine alkaloids), アルカロイド化合物(Simple piperidine alkaloids)
[構造式]

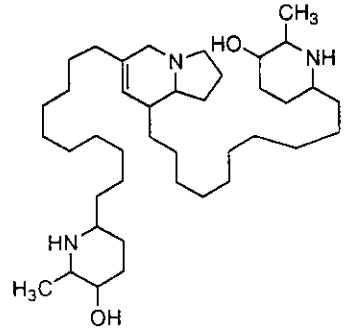


[分子式]$C_{40}H_{75}N_3O_2$
[分子量]630.051
[基原]次の植物から得られるアルカロイド: *Prosopis juliflora* の葉(マメ科)
[用途]抗菌作用を示す
[性状]ガム
[比旋光度]:[α]$_D$ +4.3 (c, 1.4 in $CHCl_3$)
[その他のデータ]Two structs. stereoisomeric with Juliflorine have been proposed but current spectroscopic data cannot distinguish between them

----------文献----------

Aqeel, A. et al., Arzneim.-Forsch., 1989, 39, 652, (性質, Julifloricine)
Ahmad, V.U. et al., J. Nat. Prod., 1989, 52, 497, (Juliflorinine)

§ Juliflorine; Stereoisomer (2)
[化学名・別名]Juliflorinine
[CAS No.]122441-92-3
[化合物分類]アルカロイド化合物(Indolizidine alkaloids), アルカロイド化合物(Miscellaneous piperidine alkaloids), アルカロイド化合物(Simple piperidine alkaloids)
[構造式]

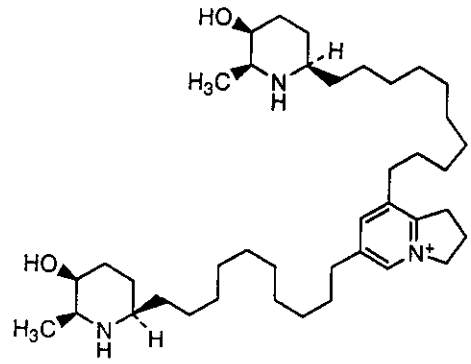


[分子式]$C_{40}H_{75}N_3O_2$
[分子量]630.051
[基原]次の植物から得られるアルカロイド: *Prosopis juliflora* の葉(マメ科)
[比旋光度]:[α]$_D$ +3.9 (c, 0.03 in $CHCl_3$)
[溶解性]BERDY SOL: メタノール, ベンゼンに可溶
UV: [neutral] λ_{max} 208; 285(MeOH) (Berdy)
[その他のデータ]Has (2α,5β,6beta) configs. of the piperidine systems

----------文献----------

Aqeel, A. et al., Arzneim.-Forsch., 1989, 39, 652, (性質, Julifloricine)
Ahmad, V.U. et al., J. Nat. Prod., 1989, 52, 497, (Juliflorinine)

§ Juliprosine
[化学名・別名]2,3-Dihydro-6,8-bis[10-(5-hydroxy-6-methyl-2-piperidinyl)decyl]-1*H*-indolizinium (CAS 名)
[CAS No.]80233-19-8
[化合物分類]アルカロイド化合物(Simple piperidine alkaloids), アルカロイド化合物(Indolizidine alkaloids)
[構造式]

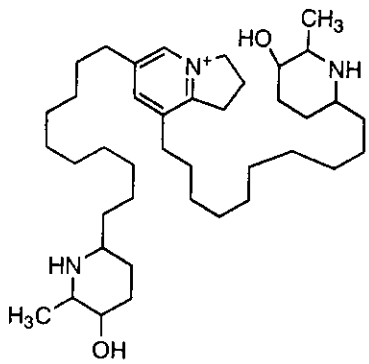


[分子式] $C_{40}H_{72}N_3O_2^{(+)}$
[分子量] 627.028
[基原] 次の植物から得られるアルカロイド: *Prosopis juliflora* (マメ科)
[性状] オイル (as chloride)
[比旋光度]: [α]$_D$ +11 (c, 0.50 in $CHCl_3$) (chloride)
[溶解性] BERDY SOL: メタノール, クロロホルムに可溶
UV: [neutral] λ $_{max}$ 279 (ε 6200) (EtOH) (Berdy)

文 献

Dätwyler, P. et al., Helv. Chim. Acta, 1981, 64, 1959, (分離, spectra)
Ahmad, A. et al., Fitoterapia, 1989, 60, 86-89, (Isojulioprosine)

§ Juliprosine; 5',5'',6',6''-Tetraepimer

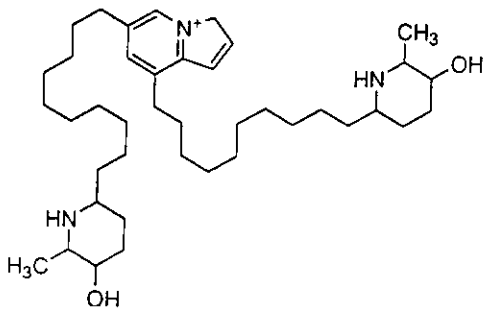


[化学名・別名] Isojuliprosine
[CAS No.] 123805-40-3
[その他の CAS No.] 123750-53-8
[化合物分類] アルカロイド化合物(Indolizidine alkaloids), アルカロイド化合物(Simple piperidine alkaloids)
[構造式]
[分子式] $C_{40}H_{72}N_3O_2^{(+)}$
[分子量] 627.028
[基原] 次の植物から得られるアルカロイド: *Prosopis juliflora* (マメ科)
[性状] 黄色のオイル (as chloride)
[溶解性] BERDY SOL: メタノール, クロロホルムに可溶
UV: [neutral] λ $_{max}$ 280 (EtOH) (Berdy)

文 献

Ahmad, A. et al., Fitoterapia, 1989, 60, 86-89, (Isojulioprosine)

§ Juliprosine; 2,3-Didehydro

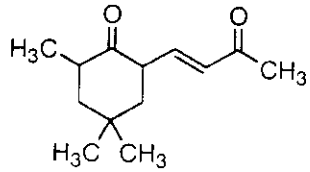


[化学名・別名] 6,8-Bis[10-(5-hydroxy-6-methyl-2-piperidinyl)decyl]-1*H*-indolizinium. Juliprosinene
[CAS No.] 123061-99-4
[化合物分類] アルカロイド化合物(Simple piperidine alkaloids), アルカロイド化合物(Miscellaneous piperidine alkaloids), アルカロイド化合物(Indolizidine alkaloids)
[構造式]
[分子式] $C_{40}H_{70}N_3O_2^{(+)}$
[分子量] 625.012
[基原] 次の植物から得られるアルカロイド: *Prosopis juliflora* の葉(マメ科)
[性状] ガム (as chloride)
[比旋光度]: [α]$_D$ +9.5 (c, 0.04 in $CHCl_3$) (chloride)
[溶解性] BERDY SOL: メタノール, ベンゼンに可溶
UV: [neutral] λ $_{max}$ 208; 285 (MeOH) (Berdy)

文 献

Ahmad, V.U. et al., J. Nat. Prod., 1989, 52, 497, (分離, UV, IR, H-NMR, C13-NMR, Mass, 構造)

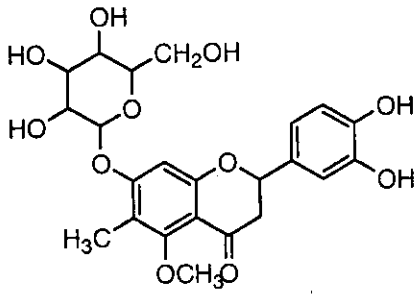
§ Prosopidione



[化学名・別名] 2,4,4-Trimethyl-6-(3-oxo-1-butenyl)cyclohexanone (CAS 名)
[CAS No.] 120166-32-7
[化合物分類] テルペノイド(Miscellaneous cyclohexane sesquiterpenoids)
[構造式]

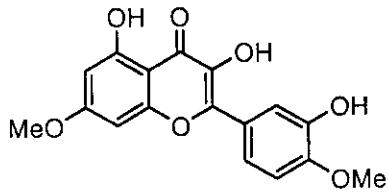
[基原]*Prosopis juliflora*
[性状]無定型の粉末
[融点]Mp 202 ℃で分解
[比旋光度]:[α]$_D$ -19.2(MeOH)
----------文献----------
Ahmad, V.U. et al., Phytochemistry, 1989, 27, 278

§ 3',4',5,7-Tetrahydroxy-6-methylflavanone; (*S*)-form, 5-Me ether, 7-*O*-β-D-glucopyranoside
[CAS No.]85687-89-4
[化合物分類]フラボノイド(Flavones), フラボノイド(Flavanones; 4 × O-置換基)
[構造式]



[分子式]$C_{23}H_{26}O_{11}$
[分子量]478.452
[基原]次の植物から分離: *Prosopis juliflora*
[性状]結晶
[融点]Mp 231 ℃
----------文献----------
Barton, G.M., Phytochemistry, 1972, 11, 426
Malhotra, S. et al., Planta Med., 1983, 47, 46
Harborne, J.B. et al., Phytochemistry, 1993, 34, 219

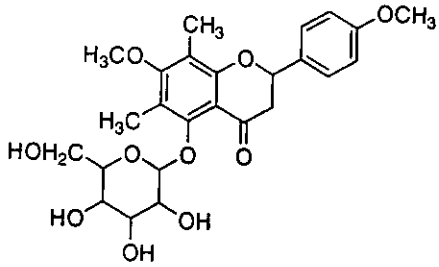
§ 3,3',5-Trihydroxy-4',7-dimethoxyflavone
[化学名・別名]3,5-Dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-7-methoxy-4*H*-1-benzopyran-4-one(CAS 名). 3',5-Dihydroxy-4',7-dimethoxyflavonol. Ombuin
[CAS No.]529-40-8
[化合物分類]フラボノイド(Flavonols; 5 × O-置換基)
[構造式]



[分子式]$C_{17}H_{14}O_7$
[分子量]330.293
[基原]*Prosopis juliflora* の樹皮, *Phytolacca dioica*, *Angelonia*, *Cassia*, *Ostrya*, *Eupatorium* spp.
[性状]黄色の結晶
[融点]Mp 230 ℃
[化学物質毒性データ総覧(RTECS)登録番号]LK8332000
----------文献----------
Hoerhammer, L. et al., Chem. Ber., 1968, 101, 1183, (Ombuoside)
Bonefeld, M. et al., Phytochemistry, 1986, 25, 1205, (Ombuoside)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988

***RTECS (化学物質毒性データ) ***
生体影響物質　　：変異原性物質.
健康障害に関するデータ
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：166 nmol/plate
参照文献
Mutation Research.(Elsevier Science Pub. B.V., POB 211, 1000 AE Amsterdam, Netherlands)54,297,1978

§ 4',5,7-Trihydroxy-6,8-dimethylflavanone; (*S*)-form, 4',7-Di-Me ether, 5-*O*-β-D-galactopyranoside
[CAS No.]85687-90-7
[化合物分類]フラボノイド(Flavanones: 3 × O-置換基)
[構造式]



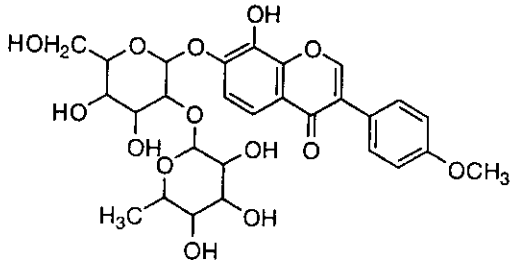
[分子式] $C_{25}H_{30}O_{10}$
[分子量] 490.506
[
正確な分子量] 490.1839
[基原] 次の植物から分離:*Prosopis juliflora* の根
[融点] Mp 195 ℃で分解

----------文 献----------

Youssef, D.T.A. et al., Phytochemistry, 1998, 49, 2579-2583, (分離, IR, H-NMR, C13-NMR)

§ 4',7,8-Trihydroxyisoflavone; 4'-Me ether, 7-*O*-[α -L-rhamnopyranosyl-(1 → 2) -β -D-glucopyranoside]

[化学名・別名] Retusin 7-neohesperidoside
[CAS No.] 78386-04-6
[化合物分類] フラボノイド(Isoflavones; 3 × O-置換基)
[構造式]



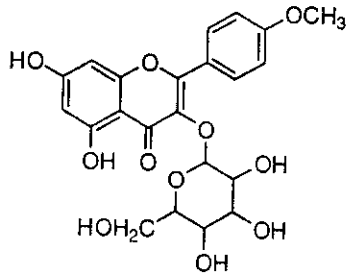
[分子式] $C_{28}H_{32}O_{14}$
[分子量] 592.552
[基原] 次の植物から分離: *Prosopis juliflora*

----------文 献----------

Karmarkar, S.S., J. Sci. Ind. Res., Sect. B, 1961, 20, 334, (合成法)
Jurd, L. et al., Tet. Lett., 1972, 2149, (Retusin)
Hayashi, T. et al., Phytochemistry, 1974, 13, 1943, (Retusin)
Mitra, J. et al., Phytochemistry, 1983, 22, 2326, (Retusin 7-glucoside)
Ingham, J.L., Prog. Chem. Org. Nat. Prod., 1983, 43, 1, (レビュー, 生育)
(H-NMR, Mass, Retusin)

§ 3,5,7-Trihydroxy-4'-methoxyflavone; 3-*O*-β-D-Galactopyranoside

[CAS No.] 78386-03-5
[化合物分類] フラボノイド(Flavonols; 4 × O-置換基)
[構造式]



[分子式] $C_{22}H_{22}O_{11}$
[分子量] 462.409
[基原] 次の植物から分離: *Prosopis juliflora*
[性状] 黄色の針状結晶(EtOAc/petrol)
[融点] Mp 168 ℃

----------文 献----------

Brandes, R., Annalen, 1839, 32, 311, (分離)
Vajpeyi, R.L. et al., Phytochemistry, 1981, 20, 339, (3-galactoside)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988

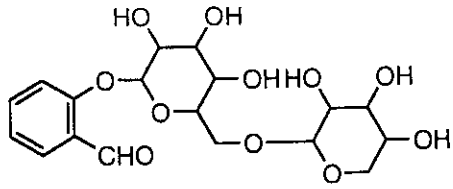
***********メドウスイート (Meadowsweet) **********

§§バラ科セイヨウナツユキソウ(*Filipendula ulmaria* (L.) Maximowicz)の全草。

§ 2-Hydroxybenzaldehyde; *O*-[β-D-Xylopyranosyl-(1 → 6)-β-D-glucopyranoside]

[化学名・別名] Spiraein ‡
[CAS No.] 14907-56-3
[化合物分類] 単環芳香族(Simple benzaldehydes)
[構造式]

[分子式] $C_{18}H_{24}O_{11}$
[分子量] 416.381
[基原] 次の植物から分離: *Spiraea kamtschatica*, *Filipendula ulmaria*

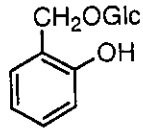


[性状] 針状結晶・一水和物 (EtOH)
[融点] Mp 230-231 ℃
[比旋光度]: $[\alpha]_D$ -57.9 (c, 1.22 in H_2O)

----------文献----------

Thieme, H., Pharmazie, 1965, 20, 113; CA, 66, 26602k, (Spiraein)

§ Isosalicin



[CAS No.] 7724-09-6
[化合物分類] 単環芳香族 (Simple benzyl alcohols)
[構造式]
[分子式] $C_{13}H_{18}O_7$
[分子量] 286.281
[基原] 次の植物から分離: flowers of *Filipendula ulmaria* の花
[性状] 針状結晶・三水和物 (Me_2CO/petrol)
[融点] Mp 66-68 ℃
[比旋光度]: $[\alpha]_D^{20}$ -45.2 (無水物)

----------文献----------

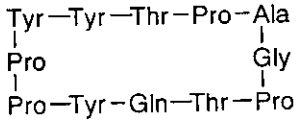
Bourquelot, E. et al., C. R. Hebd. Seances Acad. Sci., 1913, 156, 1790, (合成法)
Thieme, H., Pharmazie, 1966, 21, 123, (分離)

§§ バラ科ロクベンシモツケ (***Filipendula hexapetala*** **Gilibert**) の全草。
本調査研究では、成分に関する文献はなかった。

*********メハジキ (Mehajiki) *********

§§ シソ科メハジキ (*Leonurus sibiricus* L.) の全草。

§ Cycloleonurinin



[CAS No.] 135447-56-2
[化合物分類] アミノ酸とペプチド (Cyclic oligo- and polypeptides)
[構造式]
[分子式] $C_{65}H_{85}N_{13}O_{18}$
[分子量] 1336.463
[一般的性質] Cyclic peptide
[基原] 次の植物から分離: *Leonurus artemisia* の果実, *Leonurus heterophyllus*, *Leonurus sibiricus*
[性状] 粉末・五水和物 (MeOH)
[融点] Mp 222-225 ℃
[比旋光度]: $[\alpha]_D$ -28.8 (c, 0.79 in MeOH)

----------文献----------

Kinoshita, K. et al., Chem. Pharm. Bull., 1991, 39, 712, (分離, H-NMR, C13-NMR, Mass)
Morita, H. et al., Tetrahedron, 1997, 53, 7469, (H-NMR, C13-NMR, conformn)

§ 9,13:15,16-Diepoxy-8-hydroxy-7-oxo-14-labden-19,16-olide; (*ent*-6 β,8 α,9 α,13*R*)-form, 8-Ac
[化学名・別名] (+)-Leosibiricin
[CAS No.] 86575-85-1
[化合物分類] テルペノイド (Labdane diterpenoids)
[分子式] $C_{22}H_{28}O_7$
[分子量] 404.459
[基原] *Leonurus sibiricus*
[性状] 不安定なオイル
[比旋光度]: $[\alpha]_D^{17}$ +33 (c, 0.09 in $CHCl_3$)

----------文 献----------
Savona, G. et al., Phytochemistry, 1982, 21, 2699, (分離, H-NMR, C13-NMR)
Tasdemir, D. et al., J. Nat. Prod., 1995, 58, 1543, (分離, H-NMR, C13-NMR)

§ 15,16-Epoxy-3,6,9,19-tetrahydroxy-13(16),14-labdadien-7-one; (3 β,6 β,8 ξ,9 α)-form, 3,19-Di-Ac
[化学名・別名]Leosibirin
[CAS No.]86575-87-3
[化合物分類]テルペノイド(Labdane diterpenoids)
[分子式]$C_{24}H_{34}O_8$
[分子量]450.528
[基原]*Leonurus sibiricus*
[性状]オイル
[比旋光度]:$[\alpha]_D^{20}$ -0.7 (c, 0.3 in $CHCl_3$)
----------文 献----------
Savona, G. et al., Phytochemistry, 1982, 21, 2699

§ 15,16-Epoxy-3,6,9,19-tetrahydroxy-13(16),14-labdadien-7-one; (3 β,6 β,8 ξ,9 α)-form, 6-Ketone, 7xi-alcohol, 3,19-di-Ac
[化学名・別名]15,16-Epoxy-3,7,9,19-tetrahydroxy-13(16),14-labdadien-6-one. Isoleosibirin
[CAS No.]86575-86-2
[化合物分類]テルペノイド(Labdane diterpenoids)
[分子式]$C_{24}H_{34}O_8$
[分子量]450.528
[基原]*Leonurus sibiricus*
[性状]オイル
[比旋光度]:$[\alpha]_D^{28}$ +7.1 (c, 0.63 in $CHCl_3$)
----------文 献----------
Savona, G. et al., Phytochemistry, 1982, 21, 2699

§ (4-Hydroxybutyl)guanidine(CAS 名)
[化学名・別名]4-Guanidino-1-butanol. 1-Guanidino-4-hydroxybutane
[CAS No.]17581-95-2
[関連 CAS No.]106936-57-6
[化合物分類]アルカロイド化合物(Miscellaneous acyclic alkaloids)
[構造式]$HN{=}C(NH_2)NH(CH_2)_3CH_2OH$
[分子式]$C_5H_{13}N_3O$
[分子量]131.177
[基原]次の植物から得られるアルカロイド: *Leonurus sibiricus*
----------文 献----------
Fishbein, L. et al., J.A.C.S., 1954, 76, 3217-3219, (合成法)
Reuter, G. et al., Pharmazie, 1971, 26, 777, (分離)

§ Leonurine
[化学名・別名]4-[(Aminoiminomethyl) amino] butyl 4-hydroxy-3,5-dimethoxybenzoate(CAS 名). 4-Guanidinobutyl syringate
[CAS No.]24697-74-3
[化合物分類]単環芳香族(Simple benzoic acids and esters)
[分子式]$C_{14}H_{21}N_3O_5$
[分子量]311.337
[基原]次の植物から得られるアルカロイド: *Leonurus artemisia* (a Chinese herbal medicine used in obstetrics), *Leonurus sibiricus* (シソ科)
[用途]Uterotonic agent
[融点]Mp 229-230 ℃
[PKa 値]p*K*, 7.9 (H_2O)
----------文 献----------
Goto, T. et al., Tet. Lett., 1962, 545, (分離)
Sugiura, S. et al., Tetrahedron, 1969, 25, 5155, (合成法)

Yeung, H.W. et al., Planta Med., 1977, 31, 51, (分離, IR, H-NMR, Mass, 構造)

**********メープル (Maple) **********

§§カエデ科サトウカエデ(*Acer saccharum* Marshall)の樹液または樹皮。
本調査研究では、成分に関する文献はなかった。

**********メリッサ (Melissa, Balm) **********

§§シソ科セイヨウヤマハッカ(*Melissa officinalis* L.)の茎葉。

§ 2-(3,4-Dihydroxyphenyl)-1,3-benzodioxole-5-carboxaldehyde; (±)-form
[化合物分類]単環芳香族(Miscellaneous aryl derivatives)
[構造式]
[分子式]$C_{14}H_{10}O_5$
[分子量]258.23
[基原]*Melissa officinalis*
[性状]無定型の淡紫色の粉末
[融点]Mp 131-137 ℃(分解)
UV: [neutral] λ_{max} 204 (ε 2712); 230 (ε 2030); 280 (ε 1628); 310 (ε 1340)(溶媒の報告はない)
----------文献----------
Tagashira, M. et al., Planta Med., 1998, 64, 555-558, (分離, UV, IR, H-NMR, C13-NMR)

§ 3-(3,4-Dihydroxyphenyl)-2-hydroxypropanoic acid; (*R*)-form, 2-*O*-(3,4-Dihydroxy-*E*-cinnamoyl)
[化学名・別名]Rosmarinic acid. Labiatenic acid. Rosemarinic acid
[CAS No.]537-15-5
[その他の CAS No.]20283-92-5
[化合物分類]薬物: 血小板凝集阻害薬(Platelet aggregation inhibiting agents), 単環芳香族(Simple phenylpropanoids), 薬物: 抗 HIV 薬(Anti-HIV agents), 薬物: 抗炎症薬(Antiinflammatory agents), 薬物: 抗血栓薬(Antithrombotic agents), 薬物: 抗ウイルス物質(Antiviral agents)
[構造式]
[分子式]$C_{18}H_{16}O_8$
[分子量]360.32
[基原] *Rosmarinus officinalis*, *Melissa officinalis*, *Momordica balsamina*, *Mentha piperita*, *Salvia officinalis*, *Teucrium scorodonia*, *Sanicula europaea*, *Coleus blumei*, *Thymus* spp., その他の植物属
[用途]抗血栓, 抗血小板作用を示す. 抗炎症薬. 抗 HIV, 抗菌, 抗カビ作用を示す; 鎮吐剤, antigenotoxic activities etc. 植物成長阻害活性
[性状]結晶・二水和物
[融点]Mp 204 ℃で分解
[比旋光度]:$[\alpha]_D^{20}$ +145
[Log P 計算値]Log P 1.01 (計算値)
UV: [neutral] λ_{max} 230 ; 329 (MeOH) (Berdy)
[傷害・毒性]50 %致死量(LD_{50})(マウス, 静脈内) 561 mg/kg
[化学物質毒性データ総覧(RTECS)登録番号]GD8990000
----------文献----------
Schopf, C. et al., Annalen, 1940, 544, 30-62, (合成法, 3-Me ether)
Kelley, C.J. et al., J.O.C., 1975, 40, 1804; 1976, 41, 449-455, (H-NMR, C13-NMR, Rosmarinic acid)
Razzaque, A. et al., Planta, 1977, 137, 287, (生合成, Rosmarinic acid)
Ellis, B.E. et al., Planta, 1979, 147, 163, (生合成, Rosmarinic acid)
Parnham, M.J. et al., Drugs of the Future, 1985, 10, 756, (レビュー, Rosmarinic acid)
Englberger, W. et al., Int. J. Immunopharmacol., 1988, 10, 729, (薬理, Rosmarinic acid)
Peake, P.W. et al., Int. J. Immunopharmacol., 1991, 13, 853, (薬理, Rosmarinic acid)
Pabsch, K. et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.), 1991, 110, 199, (合成法, Rosmarinic acid)
Mahmood, N., Antiviral Chem. Chemother., 1993, 4, 235, (anti-HIV activity, NMR, Mass, Rosmarinic acid)

Zou, Z.W. et al., Yaoxue Xuebao, 1993, 28, 241, (薬理, Rosmarinic acid)
Abraham, S.K., Food Chem. Toxicol., 1996, 34, 15-20, (活性, Rosmarinic acid)
Binutu, O.A. et al., Planta Med., 1996, 62, 352-353, (活性, Rosmarinic acid)
Robinson, W.E. et al., Proc. Natl. Acad. Sci. U.S.A., 1996, 93, 6326-6331, (活性, Rosmarinic acid)
Eicher, T. et al., Synthesis, 1996, 755, (合成法, Rosmarinic acid)
Bogucki, D.E. et al., Can. J. Chem., 1997, 75, 1783-1794, (合成法, Rosmarinic acid)
Reimann, E. et al., Monatsh. Chem., 1997, 128, 995-1008; 1998, 129, 187-193, (合成法, Rosmarinic acid)
Kusano, G. et al., Biol. Pharm. Bull., 1998, 21, 997-999, (活性, Rosmarinic acid)

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　　：静脈内投与.

被験動物　　：げっ歯類-マウス.

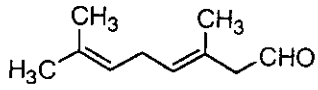
投与量・期間：561 mg/kg

毒性影響　　：致死量以外に毒性影響に関する報告はない.

Drugs of the Future.(J.R. Prous, S.A., Apartado de Correos 540, 08080 Barcelona, Spain) 10,756,1985

§ 3,7-Dimethyl-3,6-octadienal

[化学名・別名]Isocitral. β-Isogeranial



[CAS No.]1754-00-3

[関連 CAS No.]55722-59-3, 72203-97-5, 72203-98-6

[構造式]

[分子式]$C_{10}H_{16}O$

[分子量]152.236

[基原]*Cymbopogon* spp., *Melissa officinalis*, *Ophrys* spp., *Origanum* spp.

[沸点]Bp_4 70 ℃

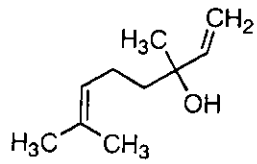
[屈折率]n^{20}_D 1.4685

文献
Sendra, J.M. et al., Phytochemistry, 1980, 19, 89-92, (分離)

§ 3,7-Dimethyl-1,6-octadien-3-ol; (*R*)-form

[CAS No.]126-91-0

[化合物分類]テルペノイド(Acyclic monoterpenoids), 薬物: 鎮静剤(Sedatives)



[構造式]

[分子式]$C_{10}H_{18}O$

[分子量]154.252

[基原]次の植物を含む精油: *Melissa officinalis* (lemon balm), ローズ, neroli, ラベンダー. *Mentha arvensis* のオイルの主成分

[用途]鎮痛, 抗菌作用を示す; active ingredient of herbal medicines containing lemon balm extracts

[性状]オイル

[沸点]Bp_{75h} 197-200 ℃

[比旋光度]:$[\alpha]_D^{20}$ -17

[Log P 計算値]Log P 2.55 (計算値)

[傷害・毒性]50 %致死量(LD_{50})(マウス, 静脈内) 180 mg/kg

[化学物質毒性データ総覧(RTECS)登録番号]RG5800000

[販売元]Fluka:62139

文献
Naves, Y.R. et al., Helv. Chim. Acta, 1963, 46, 1056; 2551, (分離, UV)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 120, (生育)
Opdyke, D.L.J., Food Chem. Toxicol., 1975, 13, 827; 833; 835; 839; 1976, 14, 459; 461; 463; 1978, 16, 811, (レビュー, 成書, esters)
Williams, P.J. et al., Phytochemistry, 1982, 21, 2013, (分離, 配糖体)
Uchiyama, T. et al., Phytochemistry, 1989, 28, 3369, (分離)
LFX000; LFY000; LFY100

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：180 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.

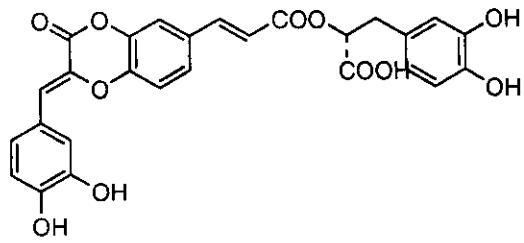
参照文献

Army Armament Research & Development Command, Chemical Systems Laboratory, NIOSH Exchange Chemicals. (Aberdeen Proving Ground, MD 21010) [Vol.,頁,年(19-)]NX#01477

米国に於ける状況

§ Melitric acid B

[CAS No.]153765-46-9
[化合物分類]単環芳香族(Simple phenylpropanoids)
[構造式]



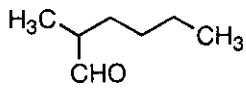
[分子式]$C_{27}H_{30}O_{11}$
[分子量]520.448
[基原]*Melissa officinalis*
[性状]淡褐色の粉末 + 1・1/2H_2O
[融点]Mp 133-135 ℃
[比旋光度]:[α]$_D^{24}$ +119.7 (c, 0.33 in MeOH)

文献

Agata, I. et al., Chem. Pharm. Bull., 1993, 41, 1608, (分離, H-NMR, C13-NMR)

§ 2-Methylhexanal; (±)-form

[CAS No.]72590-78-4
[化合物分類]脂肪族化合物(Branched aliphatic aldehydes and ketones)
[構造式]



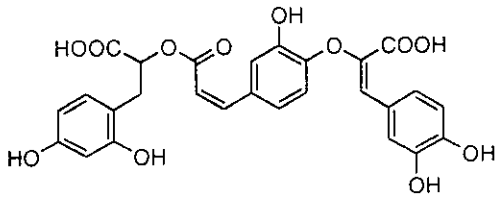
[分子式]$C_7H_{14}O$
[分子量]114.187
[基原]lemon balm, *Melissa officinalis* の精油の微量成分
[性状]液体
[沸点]Bp 141 ℃, Bp$_{60}$ 132 ℃

文献

Nykanen, I., Dev. Food Sci., 1985, 10, 329; CA, 103, 121905c, (分離)

§ Salvianolic acid I; 8''Z-Isomer

[化学名・別名]Melitric acid A. Schizotenuin E
[CAS No.]153765-45-8
[化合物分類]リグナン化合物(Neolignans), 単環芳香族(Dimeric unchlorinated depsides)
[構造式]



[分子式]$C_{27}H_{22}O_{12}$
[分子量]538.464
[基原]*Melissa officinalis*, *Salvia officinalis*, *Schizonepeta tenuifolia*
[性状]淡褐色の粉末 + 1/2H_2O
[融点]Mp 135-138 ℃
[比旋光度]:[α]$_D^{23}$ +45 (c, 0.2 in MeOH)
UV: [neutral] λ $_{max}$ 290 (log ε 4.32); 328 (log ε 4.34) (MeOH)
[その他のデータ]化学構造は Rosmarinic acid と似ている

文献

Agata, I. et al., Chem. Pharm. Bull., 1993, 41, 1608, (Melitric acid A)
Lu, Y. et al., Phytochemistry, 1999, 52, 1149-1152, (Melitric acid A)