

Dictionary
of
Organic
Compounds

SIXTH EDITION

VOLUME FIVE

Mes-Phi

0057382

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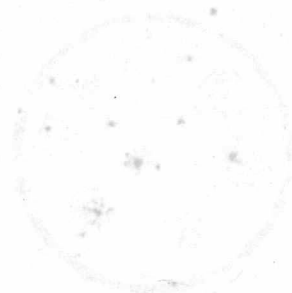
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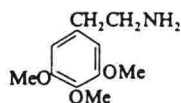
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The specific information in this publication on the hazardous and toxic properties of certain substances is included to alert the reader to possible dangers associated with the use of those compounds. The absence of such information should not however be taken as an indication of safety in use or misuse.

Mescaline**M-0-00455**

3,4,5-Trimethoxybenzeneethanamine, 9CI.
3,4,5-Trimethoxyphenethylamine. *Mezcaline*.
TMPEA
[54-04-6]



$C_{11}H_{17}NO_3$ M 211.2

Alkaloid from mescal (*Lophophora williamsii*), *Trichocereus* spp., *Gymnocalycium gibbosum*, *Opuntia cyclindrica* and other spp. in the Cactaceae. Hallucinogen; a psychotomimetic agent. Mp 35–36°. Bp₁₂ 180°.

- Adverse systemic effects by ingestion etc. esp. on CNS. LD₅₀ (mus, orl) 880 mg/kg, exp. reprod. and teratogenic effects. SI2625000.

Hydrochloride: [832-92-8].

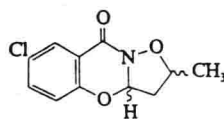
Mp 184°.

- LD₅₀ (mus, orl) 912 mg/kg. SI2800000.

Heffter, A., *Ber.*, 1896, 29, 216 (*isol*)
Späth, E. *et al.*, *Ber.*, 1937, 70, 2446; 1938, 71, 1275 (*Acetylmescaline*, *Methylmescaline*)
Reti, L. *et al.*, *J.A.C.S.*, 1951, 73, 1767 (*Trichocereine*)
Bahnholzer, K. *et al.*, *Helv. Chim. Acta*, 1952, 35, 1577 (*synth*)
Kapadia, G.J. *et al.*, *Chem. Comm.*, 1968, 1688 (*Formylmescaline*)
Kapadia, G.J. *et al.*, *J. Pharm. Sci.*, 1970, 59, 1699 (*rev*)
Lundström, J., *Acta Chem. Scand.*, 1971, 25, 3489 (*biosynth*)
Kapadia, G.J. *et al.*, *J. Pharm. Sci.*, 1977, 61, 1172 (*deriv pmr, ms*)
Smith, T.A., *Phytochemistry*, 1977, 16, 9 (*occur, rev*)
Doetsch, P.W. *et al.*, *J. Chromatogr.*, 1980, 189, 79 (*occur*)
Van Peteghem, C. *et al.*, *Eur. J. Drug Metab. Pharmacokinet.*, 1982, 7, 1 (*pharmacol*)
Bailey, K. *et al.*, *Org. Magn. Reson.*, 1983, 21, 391 (*cmr*)
Martindale, *The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, London, 1993, 1388.
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MD1500, MD1750.

Meseclazone, USAN, INN**M-0-00456**

7-Chloro-3,3a-dihydro-2-methyl-2H,9H-isoxazolo[3,2-b][1,3]benzoxazin-9-one, 9CI.
8CI. 2-Methylseclazone. W 2395
[29053-27-8]



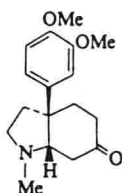
$C_{11}H_{10}ClNO_3$ M 239.6

Antiinflammatory, analgesic, antipyretic.
Cryst. (EtOAc). Mp 147–149°.

- LD₅₀ (rat, orl) 1160 mg/kg. NY3200000.
Sofia, R.D. *et al.*, *Eur. J. Pharmacol.*, 1974, 26, 51 (*pharmacol*)
Reisner, D.B. *et al.*, *Arzneim.-Forsch.*, 1977, 27, 760 (*synth, pharmacol*)
Dromgoole, S.H. *et al.*, *Drug Metab. Dispos.*, 1978, 6, 102 (*metab*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, CIL500.

Mesembrine**M-0-00457**

3a-(3,4-Dimethoxyphenyl)octahydro-1-methyl-6H-indol-6-one, 9CI. *Mesembranone*



Absolute
configuration

$C_{17}H_{23}NO_3$ M 289.3

(–)-form [24880-43-1]

Alkaloid from *Sceletium tortuosum* and *S. namaquense* (Aizoaceae). Liq. Bp_{0.3} 186–190°. $[\alpha]_D^{20}$ –55.4 (MeOH).

Hydrochloride: Mp 204.5–206° dec. $[\alpha]_D$ –8.8 (c, 0.632 in MeOH).

Deoxo: [510-80-5]. *Mesembrane*

$C_{17}H_{23}NO_2$ M 275.3 Minor alkaloid from *S. namaquense* (Aizoaceae). Oil.

6α-Alcohol: [23544-42-5]. *Mesembranol*, *Mesembrinol*

$C_{17}H_{25}NO_3$ M 291.3 Alkaloid from *S. tortuosum* and *S. strictum* (Aizoaceae), also obt. by reduct. of (–)-Mesembrine. Mp 144–145°. $[\alpha]_D$ –32 (CHCl₃).

6α-Alcohol, N-De-Me: N-*Demethylmesembranol*

$C_{16}H_{23}NO_3$ M 277.3 Alkaloid from *S. strictum* (Aizoaceae). Mp 175–185°. $[\alpha]_D$ –13.

(+)-form [468-53-1]

Synthetic. Pale-yellow oil. $[\alpha]_D^{20}$ +16.1 (c, 1.32 in MeOH).

Hydrochloride: Needles (2-propanol). Mp 208–210.5°. $[\alpha]_D^{20}$ +7.3 (c, 0.465 in MeOH).

(±)-form [6023-73-0]

Synthetic. Oil. Bp_{0.07} 178°.

Hydrochloride: Mp 179–181°.

Picrate: Cryst. (EtOH/EtOAc). Mp 171.5–172.5°.

Epimer: [21104-37-0]. 9α-Mesembrine

Synthetic. Cryst. (Et₂O/hexane). Mp 95–97°.

Epimer; hydrochloride: Mp 223–225° dec.

Popelak, A. *et al.*, *Naturwissenschaften*, 1960, 47, 156, 231 (*struct*)

Smith, E. *et al.*, *Chem. Ind. (London)*, 1961, 402 (*Mesembranol*)

Stevens, R.V. *et al.*, *J.A.C.S.*, 1968, 90, 5580 (*synth, ir, pmr*)

Keely, S.L. *et al.*, *J.A.C.S.*, 1968, 90, 5584 (*synth*)

Jeffs, P.W. *et al.*, *J.A.C.S.*, 1969, 91, 3831 (*abs config*)

Oh-ishi, T. *et al.*, *Chem. Pharm. Bull.*, 1970, 18, 299 (*synth, ir, pmr*)

Otani, G. *et al.*, *Chem. Pharm. Bull.*, 1973, 21, 2130 (*synth, cd, ord, abs config*)

Capps, T.M. *et al.*, *J.C.S. Perkin 2*, 1977, 1098 (*isol, uc, pmr, ms, cryst struct, Mesembrane*)

Jeffs, P.W. *et al.*, *Phytochemistry*, 1978, 17, 719 (*biosynth*)

Martin, S.F. *et al.*, *J.O.C.*, 1979, 44, 3391 (*synth*)

Strauss, H.F. *et al.*, *Tet. Lett.*, 1979, 4495 (*synth*)

Takano, S. *et al.*, *Tet. Lett.*, 1981, 4479 (*synth*)

Keck, G.E. *et al.*, *J.O.C.*, 1982, 47, 1302 (*synth*)

Jeffs, P.W. *et al.*, *J.O.C.*, 1983, 48, 3861 (*synth*)

Sánchez, I.H. *et al.*, *Tet. Lett.*, 1983, 24, 551 (*synth*)

Howard, A.S. *et al.*, *Tet. Lett.*, 1983, 24, 829 (*synth*)

Kochhar, K.S. *et al.*, *Tet. Lett.*, 1983, 24, 4785 (*synth*)

Meyers, A.I. *et al.*, *J.A.C.S.*, 1985, 107, 7776 (*synth*)

Gramain, J.-C. *et al.*, *Tet. Lett.*, 1985, 26, 4083 (*synth*)

Hackett, S. *et al.*, *J.O.C.*, 1986, 51, 1629 (*synth*)

Hoshino, O. *et al.*, *Chem. Pharm. Bull.*, 1987, 35, 2734 (*synth, ir, pmr*)

Winkler, J.D. *et al.*, *J.A.C.S.*, 1988, 110, 4831 (*synth*)

Shono, T. *et al.*, *Chem. Lett.*, 1989, 1963 (*synth*)

Takano, S. *et al.*, *Chem. Lett.*, 1990, 1239 (*synth*)

Bauermeister, S. *et al.*, *J.C.S. Perkin 1*, 1991, 561 (*synth*)

Parkinson, C.J. *et al.*, *J.C.S. Perkin 1*, 1991, 1053 (*synth*)

Ishibashi, H. *et al.*, *J.O.C.*, 1991, 56, 95 (*synth, Mesembranol*)

Gelas-Mialhe, Y. *et al.*, *Heterocycles*, 1992, 34, 37 (*synth*)

Michael, J.P. *et al.*, *Tet. Lett.*, 1992, 33, 6023 (*synth*)

Yokomatsu, T.Y. *et al.*, *Tet. Lett.*, 1992, 33, 6999 (*synth*)

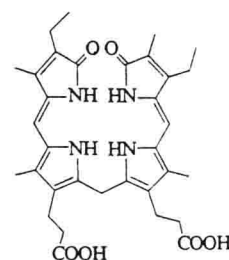
Matsumura, Y. *et al.*, *Tetrahedron*, 1993, 49, 8503 (*synth*)

Kosugi, H. *et al.*, *Tetrahedron: Asymmetry*, 1993, 4, 1409 (*synth*)

Chida, N. *et al.*, *Chem. Comm.*, 1994, 901 (*synth, Mesembranol*)

Mesobilirubin IXα**M-0-00458**

[16568-56-2]



$C_{33}H_{40}N_4O_6$ M 588.7

Obt. by partial reduction of Bilirubin, B-0-02192 or synthesis. Orange cryst. (Py or CHCl₃). Mp 315° dec.

Di-Me ester: [30046-67-4].

$C_{35}H_{44}N_4O_6$ M 616.7 Orange-red cryst. Mp 240°.

Di-Me ether:

$C_{35}H_{44}N_4O_6$ M 616.7 Formed by methylation on amide oxygens. Orange-red cryst. Mp 212°.

Di-Me ester, di-Me ether:

$C_{37}H_{48}N_4O_6$ M 644.8 Orange-red cryst. Mp 190°.

Siedel, W., *Hoppe Seyler's Z. Physiol. Chem.*, 1937, 245, 257 (*synth*)

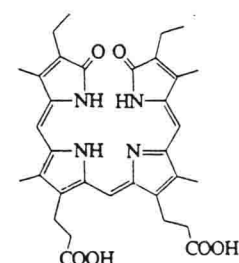
Crook, P.J. *et al.*, *Annalen*, 1971, 748, 26.

Monti, D. *et al.*, *Gazz. Chim. Ital.*, 1982, 112, 367 (*synth*)

Mesobiliverdin IIIα**M-0-00459**

Glauco bilin IIIα

[29973-74-8]



$C_{33}H_{38}N_4O_6$ M 586.6

Di-Me ester: [29789-75-1].

$C_{35}H_{42}N_4O_6$ M 614.7 Violet-blue
cryst. ($CHCl_3$). Mp 237.5-238.5°.

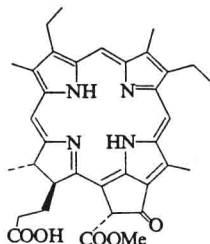
Siedel, W. *et al*, *Hoppe Seyler's Z. Physiol. Chem.*, 1933, 237, 8.

Stoll, M.S. *et al*, *Biochem. J.*, 1977, 163, 59
(*synth*, *pmr*, *ms*)

Mesophaeophorbide a

M-0-00460

Dihydrophaeophorbide a



$C_{35}H_{38}N_4O_5$ M 594.7

Prepd. by controlled catalytic hydrogenation
of Phaeophorbide a, P-0-00881. Grey
solid. Sol. $CHCl_3$. $[\alpha]_D^{20}$ -181 (Me_2CO).

Me ester: [34278-95-0]. *Methyl
dihydrophaeophorbide a*

$C_{36}H_{40}N_4O_5$ M 608.7 Prepd. by
catalytic reduction of the corresponding
methyl ester of Phaeophorbide a, P-0-
00881. Grey-black cryst. (Et_2O /hexane).
Mp 241°. $[\alpha]_D^{20}$ -180 (Me_2CO).

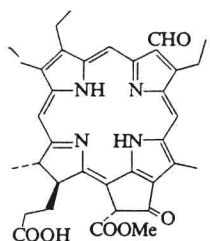
Fischer, H. *et al*, *Annalen*, 1934, 509, 269.

Fischer, H. *et al*, *Die Chemie des Pyrrols*,
Akademische Verlag, Leipzig, Vol. II, (ii),
1940, 67 (*synth*)

Jackson, A.H. *et al*, *Tetrahedron*, 1965, 21, 2913
(*ms*)

Mesophaeophorbide b

M-0-00461



$C_{35}H_{36}N_4O_6$ M 608.6

Prepd. by careful reduction of
Phaeophorbide b, P-0-00882. Important
compd. in the structural elucidation of
Chlorophyll b, C-0-03165. Grey-black
solid (CH_2Cl_2 /MeOH). Sol. $CHCl_3$. $[\alpha]_D^{20}$
-128 (Me_2CO).

Me ester: [5522-72-5].

$C_{36}H_{38}N_4O_6$ M 622.7 Blue-black solid
(Et_2O). $[\alpha]_D^{20}$ -388 (Me_2CO).

Fischer, H. *et al*, *Die Chemie des Pyrrols*,
Akademische Verlag, Leipzig, Vol. II, (ii),
1940, 249 (*synth*)

Jackson, A.H. *et al*, *Tetrahedron*, 1965, 21, 2913
(*ms*)

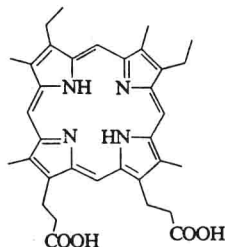
Smith, K.M. *et al*, *Tetrahedron*, 1975, 31, 367
(*cmr*)

Mesoporphyrin IX

M-0-00462

3,8-Diethyl-2,7,12,18-tetramethylporphyrin-
13,17-dipropionic acid. 2,4-Diethyl-1,3,5,8-
tetramethylporphyrin-6,7-dipropionic acid
(*obsol.*)

[493-90-3]



$C_{34}H_{38}N_4O_4$ M 566.6

Occurs in trace amounts in faeces, obt. from
Haemin, H-0-00006 or 3-Hydroxy-4-*tert*-
butylcyclohexanecarboxylic acid, H-0-
01892 by reduction. Red-violet cryst.
(Et_2O /AcOH). Mp >270° dec.

Di-Me ester: [1263-63-4].

$C_{36}H_{42}N_4O_4$ M 594.7 Purple cryst.
($CHCl_3$ /MeOH). Mp 216°.

Fe complex: [18040-04-5]. *Mesohaem. Iron
mesoporphyrin*

$C_{34}H_{36}FeN_4O_4$ M 620.5 Isol. from
various coals.

Sn complex: [122507-14-6]. *Tin
mesoporphyrin*

$C_{34}H_{34}SnN_4O_4$ M 681.3 Haem
oxygenase inhibitor.

Aldrich Library of FT-IR Spectra, 1st edn., 2,
574D (*ir*)

Fischer, H. *et al*, *Die Chemie des Pyrrols*,
Akademische Verlag, Leipzig, Vol. II, 1937
(i)

Jackson, A.H. *et al*, *J.C.S.(C)*, 1967, 2045.

Little, R.G. *et al*, *J.A.C.S.*, 1975, 97, 5363 (*cryst
struct*)

Fuhrhop, J.-H. *et al*, *Laboratory Methods in
Porphyrin and Metalloporphyrin Research*,
Elsevier, Amsterdam, 1975, 17.

Janson, T.R. *et al*, *The Porphyrins*, (Dolphin,
D., Ed.), Academic Press, N.Y., Vol. IV,
1979, 1 (*nmr*)

Dinello, R.K. *et al*, *The Porphyrins*, (Dolphin,
D., Ed.), Academic Press, N.Y., Vol. I, 1979,
289.

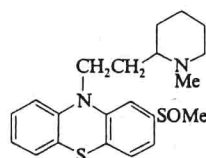
Bonnett, R. *et al*, *Chem. Comm.*, 1983, 1085
(*Mesohaem*)

Drummond, G.S. *et al*, *Arch. Biochem. Biophys.*,
1987, 255, 64 (*Sn complex*)

Mesoridazine, BAN, USAN, INN M-0-00463

10-[2-(1-Methyl-2-piperidiny)ethyl]-
2(methylsulfinyl)-10H-phenothiazine, 9CI.
Calodal

[5588-33-0]



$C_{21}H_{26}N_2OS_2$ M 386.5

Stereochem. undefined. Tranquilliser.

Oxidative metabolite of Thioridazine, T-0-
03381. Oil.

► LD₅₀ (rat, orl) 664 mg/kg. SP1880000.

Tartrate: [15296-00-1].

Cryst. ($EtOAc$). Mp 115-120°.

Benzenesulfonate (1:1): [32672-69-8].

Mesoridazine besylate, USAN. *Lidanar*.

Lidanil. *Lidanor*. *Serentil*. NC 123

► DB7176700.

U.S. Pat., 3 084 161, (1963); CA, 59, 10072a
(*synth*)

Loew, D.M. *et al*, *Boll. Chim. Farm.*, 1967, 106,
332 (*pharmacol*)

Coombs, R.A., *Arch. Mass Spectral Data*, 1971,
2, 754 (*ms*)

Ng, C.H. *et al*, *Br. J. Clin. Pharmacol.*, 1977, 4,
173; CA, 87, 47856v (*glc*)

Gershon, S. *et al*, *J. Clin. Psychiatry*, 1981, 42,
463 (*rev*, *pharmacol*)

Whelpton, R. *et al*, *J. Chromatogr.*, 1988, 426,
223 (*resoln*, *hplc*)

Martindale, The Extra Pharmacopoeia, 30th
edn., Pharmaceutical Press, London, 1993,
603.

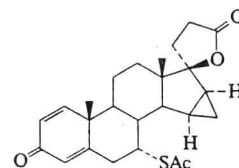
Lewis, R.J., *Sax's Dangerous Properties of
Industrial Materials*, 8th edn., Van Nostrand
Reinhold, 1992, MON750.

Mespirenone, INN

M-0-00464

ZK 94679

[87952-98-5]



$C_{25}H_{30}O_4S$ M 426.5

Aldosterone antagonist. Cryst. (MeOH). Mp
281°. $[\alpha]_D^{20}$ -82.3 ($CHCl_3$).

Hildebrand, M. *et al*, *J. Chromatogr.*, 1987, 414,
217 (*hplc*)

Nickisch, K. *et al*, *J. Med. Chem.*, 1987, 30,
1403 (*synth*, *pharmacol*)

Hildebrand, M. *et al*, *Xenobiotica*, 1987, 17, 623
(*metab*)

Mesterolone, BAN, USAN, INN M-0-00465

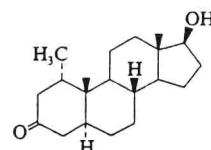
17β-Hydroxy-1α-methyl-5α-androstan-3-one.

Androviron. *Dapoder*. *Gavrol*. *Gavrolin*.

Mestoranum. *Pro-viron*. *Sten-or*. *Testiwop*.

Vistimon. NSC 75054. SH 60723

[1424-00-6]



$C_{26}H_{32}O_2$ M 304.4

Androgen. Cryst. ($EtOAc$). Mp 203.5-205°.

$[\alpha]_D^{20}$ +17.6 (c, 0.9 in $CHCl_3$).

► BV8063400.

Huck, H. *et al*, *Wien. Klin. Wochenschr.*, 1972,
84, 114 (*metab*)

Mori, H. *et al*, *Chem. Pharm. Bull.*, 1975, 23,
980.

Baran, L. *et al*, *Pol. J. Pharmacol. Pharm.*,
1981, 33, 299 (*pharmacol*)

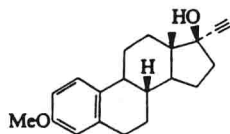
Martindale, The Extra Pharmacopoeia,
28th/29th edn., Pharmaceutical Press,
London, 1982/1989, 9064.

Laurent, H. *et al*, *Annalen*, 1983, 1996 (*synth*)

Danaci, S. *et al*, *Acta Cryst. C*, 1988, 44, 1677
(*cryst struct*)

Mestranol, BAN, USAN**M-0-00466**

3-Methoxy-19-norpregna-1,3,5(10)-trien-20-yn-17-ol, 9CI. 17 α -Ethynyl-3-methoxy-1,3,5(10)-estratrien-17 β -ol. Devocin. Ovastol. Tranel. CB 8027. EE₃ME. L 33355. RS 1044 [72-33-3]

C₂₁H₂₆O₂ M 310.4

Widely-used estrogen. Used in combination as an oral contraceptive. Cryst. (Me₂CO). Mp 150-151°. [α]_D +2 (c, 1.0 in dioxan). Component of Ortho-Novin, Femigen and Norbiogest.

► RC8960000.

17-Epimer: Epimestranol

Cryst. Mp 139.5-140°. [α]_D²⁰ +71.3 (CH₂Cl₂).

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 3, 591A (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 2, 1056B (ir)

Colton, F.B. *et al*, J.A.C.S., 1957, 79, 1123 (synth)

Smith, D.H. *et al*, Tetrahedron, 1973, 29, 3117 (ms)

Ranney, R.E. *et al*, J. Toxicol. Environ. Health, 1977, 3, 139 (rev, metab)

Horvath, G. *et al*, Adv. Mass Spectrom., 1978, 7B, 1280 (ms)

Kanojia, R.M. *et al*, J. Med. Chem., 1979, 22, 1538 (synth, pharmacol)

Wachter, M.P. *et al*, Steroids, 1979, 33, 287 (pmr, struct)

Westmijze, H. *et al*, Tet. Lett., 1980, 2665 (synth)

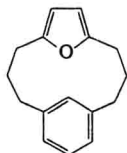
El-Obeid, H.A. *et al*, Anal. Profiles Drug Subst., 1982, 11, 375 (rev)

Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, London, 1982/1989, 9065.

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, MKB750.

[3]Metacyclo(2,5)[3]furanophane**M-0-00467**

[100994-39-6]

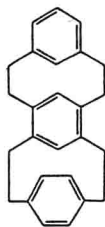
C₁₆H₁₈O M 226.3

Plates by subl. Mp 51.5-52.5°.

Shinmyozu, T. *et al*, J.O.C., 1986, 51, 1551 (synth, pmr)

[2.2]Metacyclo(4,6)[2.2]metaparacyclophane**M-0-00468**

Pentacyclo[17.2.2.1^{4,16}.1^{5,15}.1^{8,12}]hexacos-4,8,10,12(26),15(25),16(24),19,21,22-nonaene, 9CI [51657-10-4]

C₂₆H₂₆ M 338.4

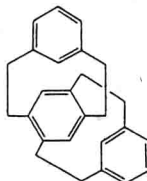
Prisms (toluene). Mp 209-210°.

Misumi, S. *et al*, Tet. Lett., 1973, 4537.

Misumi, S. *et al*, Bull. Chem. Soc. Jpn., 1976, 49, 3203, 3208.

[2.2]Metacyclo(12,15)[2.2]metaparacyclophane**M-0-00469**

Pentacyclo[19.3.1.1^{9,13}.0^{4,16}.0^{6,18}]hexacos-1(25),4,6(18),19,11,13(26),16,21,23-nonaene, 9CI [51657-02-4]

C₂₆H₂₆ M 338.4Plates (C₆H₆/EtOH). Mp 170-171°.

[51744-07-1]

Misumi, S. *et al*, Tet. Lett., 1973, 4537.

Misumi, S. *et al*, Bull. Chem. Soc. Jpn., 1976, 49, 3203, 3208.

[2.2]Metacyclo(4,7)[2.2]paracyclophane**M-0-00470**

Pentacyclo[19.2.2.1^{9,13}.0^{4,16}.0^{6,18}]hexacos-4,6(18),9,11,13(26),16,21,23,24-nonaene, 9CI [51657-01-3]

C₂₆H₂₆ M 338.4

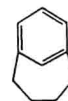
Plates (EtOH). Mp 144-145°.

Misumi, S. *et al*, Tet. Lett., 1973, 4537; 1974, 501 (synth)

Misumi, S. *et al*, Bull. Chem. Soc. Jpn., 1976, 49, 3203, 3208 (pmr, uv)

[4]Metacyclophane**M-0-00471**

Bicyclo[4.3.1]deca-1(10),6,8-triene, 9CI [107575-48-4]

C₁₀H₁₂ M 132.2

Reactive intermediate, generated by thermolysis of its Dewar isomer; it gives a mixt. of [2+2] and [4+2] dimers.

Kostermans, G.B.M. *et al*, J.A.C.S., 1987, 109, 7887.

[5]Metacyclophane**M-0-00472**

Bicyclo[5.3.1]undeca-1(11),7,9-triene, 9CI [7124-97-2]

C₁₁H₁₄ M 146.2

Liq.

v. Straten, J.W. *et al*, Tet. Lett., 1977, 4667 (synth)

Turkenburg, L.A. *et al*, Tet. Lett., 1981, 3317 (synth)

Turkenburg, L.A.M. *et al*, Tet. Lett., 1983, 24, 1821 (pmr)

Jenneskens, L.W. *et al*, J.C.S. Perkin 2, 1989, 1893 (struct)

[6]Metacyclophane**M-0-00473**

Bicyclo[6.3.1]dodeca-1(12),8,10-triene, 9CI [7125-01-1]

C₁₂H₁₆ M 160.2

Liq.

Hirano, S. *et al*, Tetrahedron, 1975, 31, 2219 (synth, pmr, ir, ms)

[7]Metacyclophane**M-0-00474**

Bicyclo[7.3.1]trideca-1(13),9,11-triene, 9CI [7125-06-6]

C₁₃H₁₈ M 174.2Liq. Bp₄ 115°.Fujita, S. *et al*, Tet. Lett., 1972, 403 (synth)

Hirano, S. *et al*, Tetrahedron, 1975, 31, 2219 (synth)

[8]Metacyclophane**M-0-00475**

Bicyclo[8.3.1]tetradeca-1(14),10,12-triene, 9CI [7048-98-8]

C₁₄H₂₀ M 188.3Tamao, K. *et al*, J.A.C.S., 1975, 97, 4405

(synth)

Bates, R.B. *et al*, J.O.C., 1982, 47, 3949 (synth, pmr)

[9]Metacyclophane**M-0-00476**

Bicyclo[9.3.1]pentadeca-1(15),11,13-triene, 9CI [7198-61-0]

C₁₅H₂₂ M 202.3Liq. Bp_{0.5} 100-105°.

Fusco, R. *et al*, Tet. Lett., 1971, 671 (synth, pmr)

Tamao, K. *et al*, J.A.C.S., 1975, 97, 4405

(synth)

Bates, R.B. *et al*, J.O.C., 1982, 47, 3949 (synth, pmr)

[10]Metacyclopentane M-0-00477

Bicyclo[10.3.1]hexadeca-1(16),12,14-triene, 9CI

[7125-13-5]

$C_{16}H_{24}$ M 216.3

Liq. Bp_{0.01} 90-100°.

Maerkl, G. *et al*, *Tet. Lett.*, 1972, 4695 (*synth*, *pmr*, *uv*)

Tamoa, K. *et al*, *J.A.C.S.*, 1975, 97, 4405 (*synth*)

Hirano, S. *et al*, *Tetrahedron*, 1975, 31, 2219 (*synth*, *pmr*, *uv*)

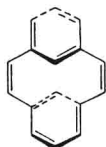
Bates, R.B. *et al*, *J.O.C.*, 1982, 47, 3949 (*synth*, *pmr*)

Higuchi, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1987, 60, 4027 (*synth*)

[2.2]Metacyclopentadiene M-0-00478

Tricyclo[9.3.1.1^{4,8}]hexadeca-1(15),2,4,6,8(16),9,11,13-octaene, 9CI

[29472-53-5]



$C_{16}H_{12}$ M 204.2

anti-form

trans-form

Cryst. Mp 119-120°. Stable indefinitely under N₂.

[673-14-3]

Mitchell, R.A. *et al*, *J.A.C.S.*, 1970, 92, 3510; 1974, 96, 1547 (*synth*, *uv*, *pmr*, *ms*)

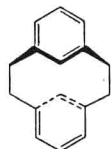
Hanson, A.W. *et al*, *Acta Cryst. B*, 1972, 28, 2032 (*cryst struct*)

Elschenbroich, C. *et al*, *Helv. Chim. Acta*, 1975, 58, 1245 (*epr*)

[2.2]Metacyclopentane M-0-00479

Tricyclo[9.3.1.1^{4,8}]hexadeca-1(15),4,6,8(16),11,13-hexaene, 9CI. Di-m-xylylene

[2319-97-3]



anti-form

$C_{16}H_{16}$ M 208.3

syn-form

Obt. in soln., characterized by *pmr*.

Isomerizes to the *anti-form* >0°.

anti-form

Stable isomer. Cryst. Mp 134.5-135°.

[51744-98-0]

Flammang, R. *et al*, *Tetrahedron*, 1968, 24, 1171 (*synth*, *pmr*, *ir*)

Kai, Y. *et al*, *Acta Cryst. B*, 1977, 33, 754 (*struct*)

Givens, R.S. *et al*, *J.O.C.*, 1979, 44, 1608 (*synth*)

Kleinschroth, J. *et al*, *Angew. Chem., Int. Ed.*, 1982, 21, 469 (*rev*)

Bates, R.B. *et al*, *J.O.C.*, 1982, 47, 3949 (*synth*)

Mitchell, R.H. *et al*, *J.A.C.S.*, 1985, 107, 3340 (*synth*, *pmr*)

[3.3]Metacyclopentane M-0-00480

Tricyclo[11.3.1.1^{5,9}]octadeca-1(17),5,7,9(18),13,15-hexaene, 9CI

[62155-71-9]

$C_{18}H_{20}$ M 236.3

Plates (EtOH). Mp 81-82°.

Shinmyozu, T. *et al*, *Chem. Lett.*, 1976, 1405 (*synth*)

Otsubo, T. *et al*, *Chem. Lett.*, 1977, 977 (*synth*, *pmr*)

Rossa, L. *et al*, *J. Chem. Res., Synop.*, 1977, 264.

Semmelhack, M.F. *et al*, *J.A.C.S.*, 1985, 107, 7508 (*synth*, *cryst struct*, *pmr*, *cmr*)

[4.2]Metacyclopentane M-0-00481

Tricyclo[11.3.1.1^{4,8}]octadeca-1(17),4,6,8(18),13,15-hexaene, 9CI

[83755-71-9]

$C_{18}H_{20}$ M 236.3

Cryst. (MeOH). Mp 43-45°.

Krois, D. *et al*, *J.C.S. Perkin 1*, 1982, 2369 (*synth*, *ir*, *pmr*)

[4.3]Metacyclopentane M-0-00482

Tricyclo[12.3.1.1^{5,9}]nonadeca-1(18),5,7,9(19),14,16-hexaene, 9CI

[83755-73-1]

$C_{19}H_{22}$ M 250.3

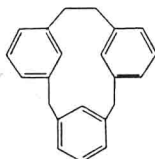
Cryst. (MeOH). Mp 28-31°.

Krois, D. *et al*, *J.C.S. Perkin 1*, 1982, 2369 (*synth*, *pmr*, *ir*)

[2.1.1]Metacyclopentane M-0-00483

Tetracyclo[14.3.1.1^{3,7}.1^{9,13}]docosa-1(20),3,5,7(22),9,11,13(21),16,18-nonaene, 9CI

[30268-90-7]



$C_{22}H_{20}$ M 284.4

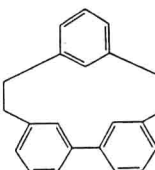
Needles. Mp 130-132°.

Sato, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1970, 43, 3632 (*synth*)

[2.2.0]Metacyclopentane M-0-00484

Tetracyclo[14.3.1.1^{2,6}.1^{9,13}]docosa-1(20),2,4,6(22),9,11,13(21),16,18-nonaene, 9CI

[24656-55-1]



$C_{22}H_{20}$ M 284.4

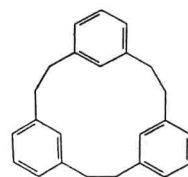
Plates (CHCl₃/MeOH). Mp 100-101°.

Vögtle, F., *Annalen*, 1969, 728, 17 (*synth*, *pmr*)

[2.2.2]Metacyclopentane M-0-00485

Tetracyclo[16.3.1.1^{4,8}.1^{11,15}]tetracosa-1(22),4,6,8(24),11,13,15(23),18,20-nonaene, 9CI. Tri-m-xylylene

[13612-55-0]



$C_{24}H_{24}$ M 312.4

Cryst. (MeOH). Mp 117-117.5°.

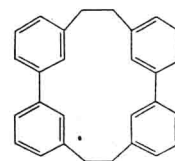
Burri, K. *et al*, *Helv. Chim. Acta*, 1967, 50, 1978 (*synth*, *ms*, *pmr*)

Flammang, R. *et al*, *Tetrahedron*, 1968, 24, 1171 (*uv*, *ir*, *pmr*, *ms*)

[2.0.2.0]Metacyclopentane M-0-00486

Pentacyclo[19.3.1.1^{2,6}.1^{9,13}.1^{14,18}]octacos-1(25),2,4,6(28),9,11,13(27),14,16,18(26),21,23-dodecaene, 9CI. [2.2](3,3')Biphenylophane

[24656-54-0]



$C_{28}H_{24}$ M 360.4

Cryst. (EtOH/C₆H₆). Mp 184-185° (174-176°).

Vögtle, F., *Annalen*, 1969, 728, 17 (*synth*)

Leach, D.N. *et al*, *J.O.C.*, 1978, 43, 2484 (*synth*, *ms*, *pmr*)

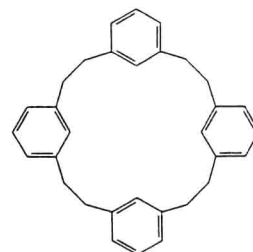
Olsson, T. *et al*, *Tetrahedron*, 1981, 37, 3473 (*pmr*)

Bates, R.B. *et al*, *Acta Cryst. C*, 1986, 42, 1199 (*cryst struct*)

[2.2.2.2]Metacyclopentane M-0-00487

Pentacyclo[23.3.1.1^{4,8}.1^{11,15}.1^{18,22}]dotriaconta-1(29),4,6,8(32),11,13,15(31),18,20,22(30),25,27-dodecaene, 9CI. Tetra-m-xylylene

[14553-78-7]



$C_{32}H_{32}$ M 416.6

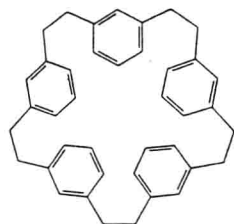
Needles (MeOH). Mp 131-131.5°.

Burri, K. *et al*, *Helv. Chim. Acta*, 1967, 50, 1978 (*synth*, *ms*, *pmr*)

Flammang, R. *et al*, *Tetrahedron*, 1968, 24, 1171 (*uv*, *ir*, *pmr*, *ms*)

[2.2.2.2]Metacyclophane M-0-00488

Hexacyclo[30.3.1.1^{4,8}.1^{11,15}.1^{18,22}.1^{25,29}]
tetraconta-1(36),4,6,8(40),11,13,15(39),18,20,
22(38),25,27,29(37),32,34-pentadecaene.
Penta-m-xylylene
[24330-20-9]

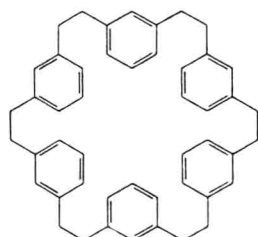


C₄₀H₄₀ M 520.7
Cryst. (MeOH). Mp 96-96.5°.

Burri, K. *et al.*, *Helv. Chim. Acta*, 1967, 50, 1978
(synth)

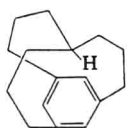
[2.2.2.2.2]Metacyclophane M-0-00489

Heptacyclo[37.3.1.1^{4,8}.1^{11,15}.1^{18,22}.1^{25,29}.1^{32,36}]
octatetraconta-1(43),4,6,8(48),11,13,15(47),
18,20,22(46),25,27,29(45),32,34,36(44),39,41-
octadecaene, 9CI. Hexa-m-xylylene
[14879-90-4]



C₄₈H₄₈ M 624.9
Needles (Me₂CO). Mp 128-129°.

Burri, K. *et al.*, *Helv. Chim. Acta*, 1967, 50,
1978, 2542 (synth, pmr, ms)

[3^{4,10}][7]Metacyclophane M-0-00490

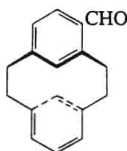
C₁₆H₂₂ M 214.3
in-form

Waxy solid.

Pascal, R.A. *et al.*, *J.A.C.S.*, 1987, 109, 6878
(synth, uv, ir, pmr)

[2.2]Metacyclophane-4-carboxaldehyde M-0-00491

4-Formyl[2.2]metacyclophane



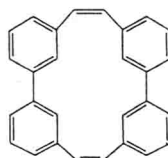
C₁₇H₁₆O M 236.3
anti-form

Solid. Mp 102-103°.

Bodwell, G.J. *et al.*, *Chem. Ber.*, 1993, 126, 167
(synth, ir, uv, pmr, cmr, ms)

[2.0.2.0]Metacyclophanediene M-0-00492

[2.2](3,3'-Biphenyl)phane-1,15-diene
[63838-45-9]

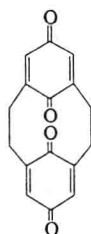


C₂₈H₂₀ M 356.4
Needles (EtOH). Mp 124-125°. λ_{max} 282 nm
(ε 19 500)(cyclohexane).

Thulin, B. *et al.*, *Tet. Lett.*, 1977, 928 (synth, uv)
Leach, D.N. *et al.*, *J.O.C.*, 1978, 43, 2484 (synth,
ms)

[2.2]Metacyclophane-5,8:13,16-diquinone M-0-00493

Tricyclo[9.3.1.1^{4,8}]hexadeca-4,7,11,14-
tetraene-6,13,15,16-tetrone, 9CI
[71777-29-2]

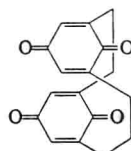


C₁₆H₁₂O₄ M 268.2
Pale-yellow prisms (Me₂CO). Mp 285-290°
dec.

Tashiro, M. *et al.*, *J.A.C.S.*, 1982, 104, 3707
(synth, uv, ir, pmr)

[3.2]Metacyclophanediquinone M-0-00494

Tricyclo[10.3.1.1^{4,8}]heptadeca-4,7,12,15-
tetraene-6,14,16,17-tetrone, 9CI



syn-form

C₁₇H₁₄O₄ M 282.2
syn-form

Yellow solid.

anti-form

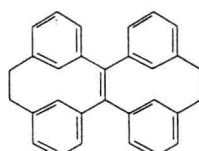
Yellow prisms (hexane). Mp 251-252°.

[143309-52-8, 143393-06-0]

Yamamoto, T. *et al.*, *J.O.C.*, 1992, 57, 5154
(synth, ir, pmr)

[0^{9,24}][2.1.2.1]Metacyclophan-9-ene M-0-00495

6,7,8,19-Tetrahydro-1,5:8,12:13,17:20,24-
tetramethenotetradecale, 9CI
[100200-62-2]



C₃₀H₂₄ M 384.5
Mp 93°. Twisted struct. of low symmetry.
Grützmacher, H.-F. *et al.*, *Tet. Lett.*, 1985, 26,
2431 (synth, pmr)

[2.2]Metacyclophan-1-ene M-0-00496

Tricyclo[9.3.1.1^{4,8}]hexadeca-
1(15),2,4,6,8(16),11,13-heptaene, 9CI
[15323-29-2]

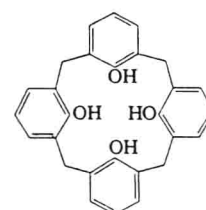


C₁₆H₁₄ M 206.2
Cryst. (EtOH).

Taylor, D., *Aust. J. Chem.*, 1978, 31, 1235 (cryst
struct)

[1.1.1.1]Metacyclophane-7,14,21,28-tetrol M-0-00497

[74568-07-3]

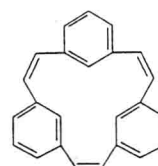


C₂₈H₂₄O₄ M 424.4
Representative of a class of compds. known
as calix[4]arenes, which adopt basket-like
conformns. and form guest-host complexes
with small molecules within the "basket".
Plates (Me₂CO). Mp 315-318°.

Gutsche, C.D. *et al.*, *J.O.C.*, 1978, 43, 4905.
Gutsche, C.D. *et al.*, *J.A.C.S.*, 1982, 104, 2652
(synth, pmr, cmr)

[2.2.2]Metacyclophanetriene M-0-00498

[89822-57-1]

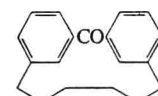


C₂₄H₁₈ M 306.4
Solid. Mp 72-75°. Bp_{0.06} 160°.

Tanner, D. *et al.*, *Acta Chem. Scand., Ser. B*,
1983, 37, 693 (synth, uv, pmr, ms)

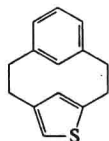
[6.1]Metacyclophan-13-one M-0-00499

[121080-14-6]

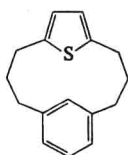


C₁₉H₂₀O M 264.3
Compds. with chain lengths of 4, 5 and 7
carbon atoms also prepd. Cryst. (MeOH).
Mp 75-77°.

Shultz, D.A. *et al.*, *J.A.C.S.*, 1989, 111, 6311
(synth, pmr, cmr, ms)

[2]Metacyclo(2,4)[2]thiophenophane
[137435-00-8]

$C_{14}H_{14}S$ M 214.3
Prisms (MeOH aq.). Mp 92-93°.
Takeshita, M. *et al*, *J.O.C.*, 1992, 57, 746
(*synth*, *ir*, *pmr*)

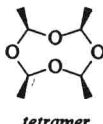
[3]Metacyclo(2,5)[3]thiophenophane
[100994-41-0]

$C_{16}H_{18}S$ M 242.3
Cryst. by subl. Mp 37-38°.
Shinmyozu, T. *et al*, *J.O.C.*, 1986, 51, 1551
(*synth*, *pmr*)

M-0-00500

Metalddehyde, BSI, ISO, JMAF M-0-00503

Helarion. Metacetaldehyde. Acetaldehyde homopolymer
[9002-91-9]



tetramer

C_2H_4O M 44.0
The tetramer is the main component and is obt. by careful crystallisation. Ordinary Metalddehyde also contains higher cyclic oligomers. Polymeric. Minimum formula given. Obt. from Acetaldehyde by polymerisation <0° in the presence of dry HCl or Py/HBr. Molluscicide.

► Flammable, fl. p. 36°. Symptoms of acute human oral tox. incl. vomiting, diarrhoea, fever, drowsiness, convulsions and coma. Death can occur. LD₅₀ (rat, orl) 227 mg/kg. Exp. reprod. effects. AB3042000.

Tetrameric-form [108-62-3]

2,4,6,8-Tetramethyl-1,3,5,7-tetroxocane, 9CI, 8CI

Cryst. with menthol odour. Needles or prisms (EtOH). Sol. most org. solvs., hot CHCl₃, spar. sol. EtOH; insol. H₂O. Mp 247°. Bp₁₃ 65°. Sublimes at 112-115° with melting. Treatment with dil. H₂SO₄ or heating in a sealed tube causes depolymerisation to acetaldehyde.

► XF9900000.

[37273-91-9]

Patterson, T.S. *et al*, *J.C.S.*, 1935, 904 (*synth*)
Pauling, L. *et al*, *J.A.C.S.*, 1936, 58, 1274 (*cryst struct*)

Craven, R.L., *J. Soc. Chem. Ind., London*, 1944, 63, 251 (*synth*)

U.S. Pat., 2 426 961, (1947); *CA*, 42, 586 (*synth*)
Frain, J., *Int. Pest Control*, 1982, 24, 150 (*rev, activity*)

Pesticide Manual, 9th edn., 1991, No. 8000.

Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A260.

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 1129.

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, TDW500.

Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1493.

Metallibure, INN

M-0-00504

N-Methyl-N'-(1-methyl-2-propenyl)-1,2-hydrazinedicarbothioamide, 9CI. *1-Methyl-6-(1-methylallyl)-2,5-dithiobiurea*, 8CI. *N-(1-Methylallylthiocarbonyl)-N'-methylthiocarbonylhydrazine. Metallibure*, BAN, USAN. Aimax. Match.
Turisyndron. AY 61122. ICI 33828. NSC 69536

[926-93-2]

$H_2C=CHCH(CH_3)NHC(S)NHNHC(S)NHMe$

$C_7H_{14}N_4S_2$ M 218.3

► LD₅₀ (rat, orl) 1000 mg/kg. Human and exp. reprod. effects. Exp. teratogen.
EC1490000.

(±)-form

Suppresses pituitary, ovarian and renal function, used mainly in animals. Mp 198-200° dec.

► EC1490000.

Loew, O., *Arch. Exp. Veterinaarmed.*, 1972, 26, 883 (*rev*)

Ger. Pat., 1 468 071, (1972); *CA*, 77, 151530p (*synth*)

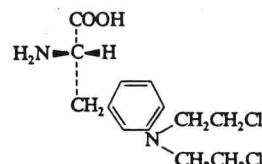
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 1388.

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MLJ500.

Metamelfalan, BAN, INN

M-0-00505

3-[Bis(2-chloroethyl)amino]phenylalanine, 9CI



$C_{13}H_{18}Cl_2N_2O_2$ M 305.2

(S)-form [1088-80-8]

Antineoplastic agent. Needles (MeOH).

Insol. H₂O. $[\alpha]_D^{25}$ -31.5.

► AY3380010.

Bergel, F. *et al*, *J.C.S.*, 1954, 2409 (*synth, pharmacol*)

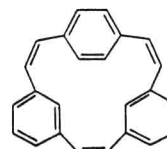
Gram, H.F. *et al*, *J. Med. Chem.*, 1963, 6, 85 (*synth, pharmacol*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, SAX210.

[2.2.2]Metametarapacyclophanetriene

M-0-00506

[89822-62-8]



$C_{24}H_{18}$ M 306.4

Cryst. Mp 127-129°.

Tanner, D. *et al*, *Acta Chem. Scand.*, Ser. B, 1983, 37, 693 (*synth, uv, pmr, ms*)

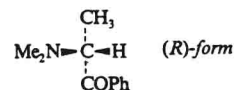
Metamfepramone, INN

M-0-00507

2-(Dimethylamino)-1-phenyl-1-propanone, 9CI. α -Dimethylaminopropiophenone. *Dimepropion*, BAN. *Effilone*. *Medulor*.

Metamfepramone. MG 559

[15351-09-4]



$C_{11}H_{15}NO$ M 177.2

► UH0539900.

(R)-form [65528-82-7]

Oil. $[\alpha]_D^{20}$ +66 (neat) (calcd).

(S)-form [35026-77-8]

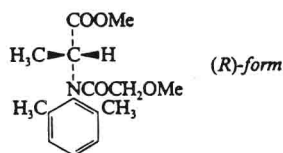
$[\alpha]_D^{25}$ -60.

Hydrochloride: Prisms. Mp 197-199°. $[\alpha]_D^{25}$ -52.5.

Metalaxyl, BSI

M-0-00502

Methyl N-(2-methoxyacetyl)-N-(2,6-dimethylphenyl)alaninate, 9CI. *Apron*. *Ridomil*. CGA 48988
[57837-19-1]



(R)-form

$C_{15}H_{21}NO_4$ M 279.3

► AY6910000.

(R)-form [70630-17-0]

More active enantiomer. Oil. $[\alpha]_D^{20}$ -55 (c, 1.89 in Me₂CO).

(±)-form

Systemic agricultural fungicide. Cryst. solid. Sol. most org. solvs.; sl. sol. H₂O. Mp 71-72°.

► LD₅₀ (rat, orl) 669 mg/kg.

U.K. Pat., 1 500 581, (1974); *CA*, 84, 30713m.

Urech, P.A. *et al*, *Phytiatr.-Phytopharm.*, 1978, 27, 239 (*rev*)

Kerkenaar, A. *et al*, *Pestic. Biochem. Physiol.*, 1981, 15, 71 (*activity*)

Fisher, D.J. *et al*, *Pestic. Sci.*, 1982, 13, 330 (*activity*)

Ripley, B.D., *J. Agric. Food Chem.*, 1985, 33, 560 (*glc, ms*)

Gozzo, F. *et al*, *Pestic. Sci.*, 1985, 16, 277 (*activity*)

Effenberger, F. *et al*, *Annalen*, 1986, 314 (*synth*)

Pesticide Manual, 10th edn., 1994, No. 452.

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MDM100.

(±)-form [65331-01-3]

Anorexic and analeptic agent. Oil. BP₁₃ 126°.

Hydrochloride: Mp 202-204°.

Picrate: Yellow needles (MeOH). Mp 128-130°.

Eidebenz, E., *Arch. Pharm. (Weinheim, Ger.)*, 1942, **280**, 49 (*synth*)

Takamatsu, H., *Yakugaku Zasshi*, 1956, **76**, 1219; *CA*, **51**, 4303 (*resoln*)

Audoye, P. *et al*, *Org. Mass Spectrom.*, 1975, **10**, 669 (*ms*)

Gaset, A., *Spectrochim. Acta A*, 1975, **31**, 727 (*ir*, *pmr*)

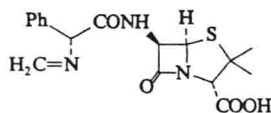
Yamamoto, K. *et al*, *Chem. Lett.*, 1977, 1115 (*resoln*, *pmr*)

Markantonis, S.L. *et al*, *Biochem. Med. Metab. Biol.*, 1989, **42**, 1 (*metab*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 1225.

Metampicillin, INN**M-0-00508**

6-[α -(Methyleneamino)phenylacetamido]penicillanic acid. *Methampicillin. Darkepen. Metalcor. Metanova. Metaval. Serfabiotic* [6489-97-0]



$C_{17}H_{19}N_3O_4S$ M 361.4

Semisynthetic penicillin (Ampicillin formaldehyde adduct). Claimed to prod. high bile concentrations.

U.K. Pat., 1 081 093, (1968); *CA*, **68**, 114595 (*synth*)

Ginocchi, G. *et al*, *Minerva Med.*, 1969, **60**, 1999, 2003, 2011 (*pharmacol*)

Sutherland, R. *et al*, *Chemotherapy*, 1972, **17**, 145 (*props*)

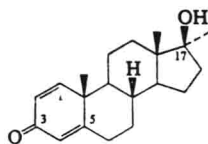
Brogard, J.M. *et al*, *J. Antimicrob. Chemother.*, 1976, **2**, 363 (*pharmacol*)

Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, Berlin, 1987, 4396 (*synonyms*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 180.

Metandienone, INN**M-0-00509**

17 β -Hydroxy-17 α -methylandrosta-1,4-dien-3-one. *1-Dehydro-17 α -methyltestosterone. Dianabol. Methandrostenolone. Vatanabol. Abirol* [72-63-9]



$C_{20}H_{28}O_2$ M 300.4

Anabolic steroid used for correction of negative nitrogen balance. Cryst. (Me_2CO/Et_2O). Mp 163-164°. [α]_D²⁵ 0 (c, 1.2 in $CHCl_3$).

► BV8000000.

Oxime: [20792-73-8].

$C_{20}H_{29}NO_2$ M 315.4 Cryst. (Me_2CO). Mp 245-250°.

Ac:

$C_{22}H_{30}O_3$ M 342.4 Cryst.

(Me_2CO /hexane). Mp 134-136°. [α]_D + 14.5 (c, 1.07 in $CHCl_3$).

[33526-40-8]

Vischer, E. *et al*, *Helv. Chim. Acta*, 1955, **38**, 1502 (*synth*)

Meystre, C. *et al*, *Helv. Chim. Acta*, 1956, **39**, 734 (*synth*)

Shapiro, E.L. *et al*, *Steroids*, 1966, **8**, 461 (*synth*)

Macdonald, B.S. *et al*, *Steroids*, 1971, **18**, 753 (*synth*, *ir*, *pmr*)

Duerbeck, H.W. *et al*, *Biomed. Mass Spectrom.*, 1980, **7**, 437 (*ms*, *metab*)

Torrini, F. *et al*, *Farmaco, Ed. Sci.*, 1980, **35**, 681 (*synth*)

Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, London, 1982/1989, 9067.

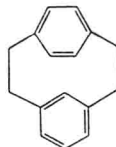
Gharavi, M. *et al*, *Int. J. Pharm.*, 1983, **14**, 325 (*props*)

Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, Berlin, 1987, 5907 (*synonyms*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DAL300.

[2.2]Metaparacyclophane**M-0-00510**

Tricyclo[9.2.2.1^{4,8}]hexadeca-4,6,8(16),11,13,14-hexaene, 9CI [5385-36-4]



$C_{16}H_{16}$ M 208.3

Cryst. Mp 81-81.5°.

Cram, D.J. *et al*, *J.A.C.S.*, 1966, **88**, 1324 (*pmr*, *uv*)

Akabori, S. *et al*, *Tet. Lett.*, 1969, 3727 (*synth*)

Hefelfinger, D.T. *et al*, *J.A.C.S.*, 1971, **93**, 4754 (*synth*)

Givens, R.S. *et al*, *J.O.C.*, 1979, **44**, 1608 (*synth*)

Higuchi, H. *et al*, *Chem. Pharm. Bull.*, 1987, **60**, 4027 (*synth*)

[3.3]Metaparacyclophane**M-0-00511**

Tricyclo[11.2.2.1^{3,9}]octadeca-5,7,9(18),13,15,16-hexaene, 9CI [64302-93-8]

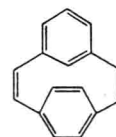
$C_{18}H_{20}$ M 236.3

Plates (hexane). Mp 90-91°.

Otsubo, T. *et al*, *Chem. Lett.*, 1977, 977 (*synth*, *pmr*)

[2.2]Metaparacyclophanediene**M-0-00512**

Tricyclo[9.2.2.1^{4,8}]hexadec-1(13),2,4,6,8(16),9,11,14-octaene, 9CI [22176-78-9]



$C_{16}H_{12}$ M 204.2

Cryst. Mp 58-59°.

Hylton, T. *et al*, *J.A.C.S.*, 1968, **90**, 6887 (*synth*)

Boekelheide, V. *et al*, *Tet. Lett.*, 1970, 1207 (*synth*)

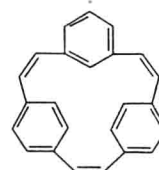
Hanson, A.W., *Acta Cryst. B*, 1971, **27**, 197 (*struct*)

Otsubo, T. *et al*, *Tet. Lett.*, 1975, 3881 (*synth*)

Bruhni, J. *et al*, *Helv. Chim. Acta*, 1990, **73**, 2058 (*epir*)

[2.2.2]Metaparaparcyclophanetriene**M-0-00513**

[89822-65-1]



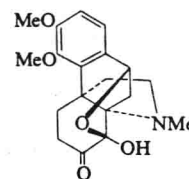
$C_{24}H_{18}$ M 306.4

Mp 75-77°.

Tanner, D. *et al*, *Acta Chem. Scand., Ser. B*, 1983, **37**, 693 (*synth*, *uv*, *pmr*, *ms*)

Metaphanine**M-0-00514**

8,10-Epoxy-8-hydroxy-3,4-dimethoxy-17-methylhasubanan-7-one, 9CI



$C_{19}H_{23}NO_5$ M 345.3

(-)-form [1805-86-3]

Alkaloid from the roots and stems of *Stephania japonica*. Also isol. from *S. abyssinica* and *S. japonica* var. *australis* (Menispermaceae). Cryst.

($Me_2CO/CHCl_3$). Mp 233°. [α]_D²⁵ -21 (c, 1.0 in $CHCl_3$). pK_a 6.03.

Hydrochloride: Cryst. + $\frac{1}{2} H_2O$ (Me_2CO). Mp 226°.

Hydroiodide: Cryst. + $\frac{1}{2} H_2O$ (THF). Mp 230° dec.

Sulfate (1:2): Cryst. + $2H_2O$ (Me_2CO). Mp 174°.

Oxime: Cryst. (Me_2CO aq.). Mp 215°.

Methiodide: Cryst. (Me_2CO /hexane). Mp 195°.

(±)-form [38305-47-4]

Synthetic. Prisms ($Et_2O/MeOH$). Mp 205-206°.

Tomita, M. *et al*, *Tet. Lett.*, 1964, 3605; 1965, 1019; *Chem. Pharm. Bull.*, 1965, **13**, 695 (*ir*, *pmr*, *ms*, *struct*)

de Waal, H.L. *et al*, *Tet. Lett.*, 1966, 6169 (*uv*, *ir*, *pmr*, *struct*)

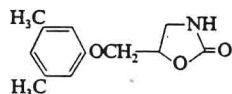
Kupchan, S.M. *et al*, *J.O.C.*, 1973, **38**, 151 (*synth*)

Ibuka, T. *et al*, *Chem. Pharm. Bull.*, 1974, **22**, 907 (*synth*, *ir*, *pmr*)

Matsui, M. *et al*, *Phytochemistry*, 1979, **18**, 1087 (*isol*)

Metaxalone, BAN, INN, USAN M-0-00515

5-[(3,5-Dimethylphenoxy)methyl]-2-oxazolidinone, 9CI. 5-(3,5-Xylyloxymethyl)oxazolidin-2-one. Metaxine. Skelaxin. AHR 438
[1665-48-1]



$C_{12}H_{15}NO_3$ M 221.2

► CNS depressant. LD₅₀ (rat, orl) 775 mg/kg. RQ3850000.

(±)-form

Muscle relaxant. Cryst. (EtOAc). Mp 121.5–123°. Bp_{1.5} 220–225°.

Lunsford, C.D. *et al*, *J.A.C.S.*, 1960, **82**, 1166 (synth)

Minyard, A. *et al*, *Tex. J. Pharm.*, 1963, **4**, 346 (pharmacol)

Sammul, O.R. *et al*, *J. Assoc. Off. Agric. Chem.*, 1964, **47**, 918 (ir)

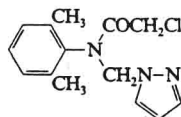
Bruce, R.B. *et al*, *J. Med. Chem.*, 1966, **9**, 286 (metab)

Martindale, *The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, London, 1993, 1205.

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, XV5000.

Metazachlor, BSI, ISO M-0-00516

2-Chloro-N-(2,6-dimethylphenyl)-N-(1H-pyrazol-1-yl)acetamide, 9CI. Butisan S [67129-08-2]



$C_{14}H_{16}ClN_3O$ M 277.7

Herbicide. Yellowish cryst. Mp 85°.

► LD₅₀ (rat, orl) 1000 mg/kg. AB5442000.

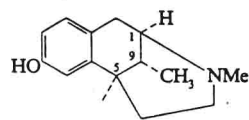
Ger. Pat., 2 828 303, (1980); *CA*, **92**, 158972c (synth, activity)

Birkler, H., *Weeds Weed Control*, 1983, **24**, 184 (activity, props, tox)

Pesticide Manual, 10th edn., 1994, No. 458.

Metazocine, BAN, INN M-0-00517

1,2,3,4,5,6-Hexahydro-3,6,11-trimethyl-2,6-methano-3-benzazocin-8-ol, 9CI. 2'-Hydroxy-2,5,9-trimethyl-6,7-benzomorphan. Methobenzorphan. NIH 7410 [3734-52-9]



(1R,5R,9R)-form

$C_{15}H_{21}NO$ M 231.3

Four stereoisomers known, of which the (1R,5R,9R)- and (1R,5R,9S)-forms are the most active physiologically. Benzomorphan numbering (illus.) is usually used. Narcotic analgesic.

(1R,5R,9R)-form [21286-60-2]

(-)-cis-form. (-)-α-form

Mp 184–186°.

Hydrobromide: Mp 248–250°.

N-De-Me: Normetazocine

$C_{14}H_{19}NO$ M 217.3 Powdery solid. Mp 261–264°. $[\alpha]_D^{25}$ –69.7 (c, 0.97 in EtOH).

N-De-Me, N-(3-methyl-2-butenyl): see

Pentazocine, P-0-00718

N-De-Me, N-(2-phenylethyl): see

Phenazocine, P-0-01134

(1S,5S,9R)-form [67009-58-9]

(β)-(+)-form

Cryst. (Me₂CO aq.). Mp 181–183°. $[\alpha]_D^{25}$ +81.8 (c, 0.83 in EtOH).

Hydrobromide: Mp 274–276° dec.

May, E.L. *et al*, *J.O.C.*, 1959, **24**, 1435 (synth)

Fullerton, S.E. *et al*, *J.O.C.*, 1962, **27**, 2144 (pmr)

Casy, A.F. *et al*, *J. Med. Chem.*, 1969, **12**, 178 (abs config, ord)

Vaughan, D.P. *et al*, *J. Pharm. Pharmacol.*, 1973, **25**, 895 (ms)

Albertson, N.F. *et al*, *J. Med. Chem.*, 1978, **21**, 471 (synth, pharmacol)

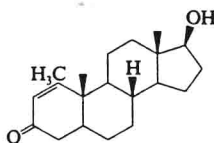
Casy, A.F. *et al*, *Org. Magn. Reson.*, 1982, **20**, 254 (cmr)

Meyers, A.I. *et al*, *J.A.C.S.*, 1985, **107**, 7974 (synth)

Brine, G.A. *et al*, *J. Het. Chem.*, 1990, **27**, 2139 (resoln)

Metenolone, INN M-0-00518

17β-Hydroxy-1-methyl-5α-androst-1-en-3-one, 9CI. Methenolone, BAN [153-00-4]



$C_{20}H_{30}O_2$ M 302.4

Anabolic steroid. Cryst. (diisopropyl ether).

Mp 149.5–152° and 159–161° (double Mp). $[\alpha]_D$ +58.9 (CHCl₃).

Me ether: 17-Methoxy-1-methylandrost-1-en-3-one

$C_{21}H_{32}O_2$ M 316.4 Mp 132–133°. $[\alpha]_D$ –39 (c, 1 in CHCl₃).

Ac: [434-05-9]. Methenolone acetate, USAN.

Metenolone acetate. Nibal. Primobolan.

Primonabol. NSC 74226. SH 567. SQ

16496

$C_{22}H_{32}O_3$ M 344.4 Anabolic steroid.

Mp 138–139° (isopropyl ether).

► BV8408500.

Heptanoyl: [303-42-4]. Methenolone

enanthate, USAN. Nibal injection.

Primobolan-Depot. NSC 64967. SH 601.

SQ 16374

$C_{27}H_{42}O_3$ M 414.6 Anabolic steroid.

[49566-70-3, 79732-38-0]

Weichert, T.R. *et al*, *Chem. Ber.*, 1960, **93**, 1710 (synth)

Popper, A. *et al*, *Arzneim.-Forsch.*, 1962, **12**, 213 (synth)

Lehmann, H.G. *et al*, *Chem. Ber.*, 1965, **98**, 1470 (synth)

Spiteller-Friedmann, M. *et al*, *Org. Mass*

Spectrom., 1968, **1**, 231 (ms)

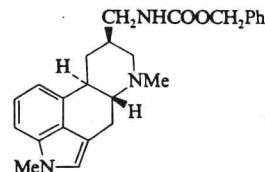
Kuhnert-Brandstaetter, *et al*, *Microchem. J.*, 1972, **17**, 719 (props, deriv)

Martindale, *The Extra Pharmacopoeia*, 28th/29th edn., Pharmaceutical Press, London, 1982/1989, 9069, 9070.

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, PMC700.

Metergoline, BAN, INN M-0-00519

[[[(8β)-1,6-Dimethylergolin-8-yl]methyl] carbamic acid phenylmethyl ester, 9CI. N-Carboxy-1-methyl-9,10-dihydrolysergamine benzyl ester. Methergoline. Al-Migren. Liserdol. FI 6337. MCE [17692-51-2]



$C_{26}H_{29}N_3O_2$ M 403.5

Analgesic, serotonin antagonist, antipyretic. Mp 168–170°.

► LD₅₀ (mus, orl) 430 mg/kg. FA1070000.

Benardi, L. *et al*, *Gazz. Chim. Ital.*, 1964, **94**, 936 (synth)

Beretta, C. *et al*, *Nature (London)*, 1965, **207**, 421, 1339 (pharmacol)

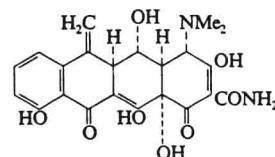
Serantoni, F. *et al*, *Acta Cryst. B*, 1977, **33**, 2899 (cryst struct)

Vicario, G.P. *et al*, *Farmaco, Ed. Sci.*, 1982, **37**, 651 (metab)

Martindale, *The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, London, 1993, 848.

Methacycline, BAN, USAN M-0-00520

4-(Dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methylene-1,11-dioxo-2-naphthacene-carboxamide, 9CI. 8CI. 6-Methyleneoxytetracycline. Bialatan. GS 2876 [914-00-1]



$C_{22}H_{22}N_2O_8$ M 442.4

Semisynthetic tetracycline antibiotic.

Prepared from Oxytetracycline by dehydration. Broad-spectrum antibiotic of limited clinical use. Mp 205° dec.

► QI9275000.

Hydrochloride: [3963-95-9]. Methacycline

hydrochloride, USAN. Randomycin

Yellow cryst. + $\frac{1}{2}$ H₂O + $\frac{1}{2}$ MeOH (MeOH aq.). Mp ca. 205° dec.

► QI9276000.

U.S. Pat., 3 026 354, (1960); *CA*, **57**, 7202 (manuf)

Blackwood, R.K. *et al*, *J.A.C.S.*, 1961, **83**, 2773; 1963, **85**, 3943 (synth, uv)

Sobiczewski, W., *Acta Pol. Pharm.*, 1975, **32**, 37; *CA*, **83**, 164498 (synth)

Asleson, G.L. *et al*, *J.A.C.S.*, 1975, **97**, 6246 (cmr)

Casy, A.F. *et al*, *J. Pharm. Biomed. Anal.*, 1983, **1**, 281 (nmr)

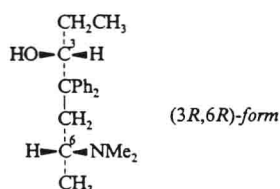
Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, Berlin, 1987, 6470 (synonyms)

Martindale, *The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, London, 1993, 180.

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MDO250.

Methadol**M-0-00521**

β -2-Dimethylaminopropyl- α -ethyl- β -phenylbenzeneethanol, 9CI. 6-Dimethylamino-4,4-diphenyl-3-heptanol, 8CI. **Dimepheptanol**, BAN, INN. Amidol†. Pangerin. NIH 2933 [545-90-4]



$C_{21}H_{29}NO$ M 311.4

Various stereoisomers of the parent alcohol and of the *O*-acetate (Methadyl acetate, BAN) are used as analgesics.

(3R,6R)-form [17199-54-1]

(+)- α -form. **Alphamethadol**, BAN, INN Cryst. Mp 100-102°.

Ac: [17199-58-5]. **Alphacetylmethadol**, INN. **Alphacemethadone**. DAAM

$C_{23}H_{31}NO_2$ M 353.5 Narcotic analgesic. Cryst. (EtOH/Et₂O). Mp 215°. [α]_D²⁵ +61.2 (c, 0.2 in EtOH).

Hydrochloride: Mp 169-171°. [α]_D²⁵ +34 (c, 0.26 in H₂O).

(3R,6S)-form [15529-92-7]

(+)- β -form

Prisms (EtOH aq.). Mp 106-107°. [α]_D²⁰ +178 (EtOH). More potent than (–)- β isomer.

Ac: Prisms. Mp 71-72°. [α]_D²⁰ +90.7 (c, 0.43 in EtOH).

Ac: hydrochloride: Needles + 1H₂O (Me₂CO aq.). Mp 158-160° (monohydrate). [α]_D²⁰ +47 (c, 0.89 in H₂O).

(3S,6S)-form [14019-10-4]

(–)- α -form. **Levomethadyl**

Analgesic. Mp 100-102°. More potent than (+)- α isomer.

Hydrochloride: Mp 169-171°. [α]_D²⁵ –34 (c, 0.3 in H₂O).

Ac: [34433-66-4]. **Levacetylmethadol**, INN. **Levomethadyl acetate**, USAN. LAAM

Ac: hydrochloride: Cryst. (EtOH/Et₂O), cryst. + 1H₂O. Mp 215° (anhyd.), Mp 159-161° (hydrate). [α]_D²⁵ –60 (c, 0.2 in EtOH).

(3S,6R)-form [17199-55-2]

(–)- β -form. **Betamethadol**, BAN, INN

Prisms. Mp 105-107°. [α]_D²⁰ –178 (EtOH). More active than the (3R,6S)-form.

▶ MJ3500000.

Ac: [17199-59-6]. **Betaacetylmethadol**, INN. **Betacemethadone**

Analgesic. Cryst. Mp 69.5-71°. [α]_D²⁰ –91.5 (c, 0.46 in EtOH).

Ac: hydrochloride: Cryst. + 1H₂O (Me₂CO/Et₂O). Mp 159-161° (206-208°). [α]_D²⁰ –46.7 (c, 0.75 in H₂O).

(3RS,6RS)-form

(±)- α -form

Analgesic. Prisms (MeOH aq.). Mp 100-100.5°.

Hydrochloride: [23164-36-5].

Prisms. Mp 192-193°.

▶ MJ3850000.

Ac: hydrochloride: Cryst. (EtOAc). Mp 213-214°.

(3RS,6SR)-form

(±)- β -form

Narcotic analgesic. Mp 127-128°.

Hydrochloride: Rods (Me₂CO). Mp 210-212°.

Ac: Cryst. (EtOH aq.). Mp 129-130°.

Ac: hydrochloride: Cryst. + $\frac{1}{2}$ or 1H₂O. Mp 142-160° (monohydrate), Mp 186-188.5° (hemihydrate).

[1477-40-3, 23164-36-5, 86360-60-3]

Bockmühl, M. et al, *Annalen*, 1948, 561, 52 (deriv)

Speeter, M.E. et al, *J.A.C.S.*, 1949, 71, 57 (deriv)

Pohland, A. et al, *J.A.C.S.*, 1949, 71, 460 (synth, resoln)

Eddy, N.B. et al, *J.O.C.*, 1952, 17, 321 (synth, pharmacol)

Portoghese, P.S. et al, *J. Pharm. Sci.*, 1966, 55, 900 (isom)

Casy, A.F. et al, *J. Med. Chem.*, 1968, 11, 601 (synth, pharmacol)

Williams, P.S. et al, *J. Med. Chem.*, 1969, 12, 839 (pmr, struct)

Shefter, E., *J. Med. Chem.*, 1974, 10, 1037 (abs config)

Archer, S., *NIDA Res. Monogr.*, 1976, 8, 10 (pharmacol, deriv)

Mule, S.J. et al, *Ann. N.Y. Acad. Sci.*, 1978, 311, 199 (pharmacol, deriv)

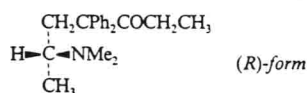
Martindale, *The Extra Pharmacopoeia*, 28th/29th edn., Pharmaceutical Press, London, 1982/1989, 6235.

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, ACQ666.

Methadone, BAN, INN**M-0-00522**

6-Dimethylamino-4,4-diphenyl-3-heptanone, 9CI, 8CI

[76-99-3]



$C_{21}H_{27}NO$ M 309.4

▶ LD₅₀ (mus, ori) 70 mg/kg. Exp. reprod. and teratogenic effects. MJ5950000.

(R)-form [125-58-6] **Levomethadone**, INN.

Levamethadone. L-Polamidon

Cryst. (2-propanol). Mp 98-100°. [α]_D²⁰ –32 (c, 1.8 in EtOH). Pharmacol. active isomer.

▶ LD₅₀ (mus, ori) 97 mg/kg. MJ5990000.

Hydrochloride: [5967-73-7]. **Levadone**

Cryst. Mp 245-246°. [α]_D²⁰ –169 (c, 2.1 in EtOH).

▶ MJ6475000.

(S)-form [5653-80-5]

Cryst. (2-propanol). Mp 100-101°. [α]_D²⁵ +26 (c, 1.5 in EtOH).

▶ LD₅₀ (mus, ori) 252 mg/kg. Exp. reprod. effects. MJ6000000.

Hydrochloride: [15284-15-8].

Cryst. (2-propanol). Mp 243-244°. [α]_D²⁵ +125 (c, 1.5 in EtOH).

▶ MJ6650000.

(±)-form [297-88-1]

Adanon. **Amidone**. **Dolophine**

Analgesic equalling morphine in potency. Used in treatment of heroin dependency (suppresses withdrawal symptoms). Cryst. (MeOH). Mp 79-81°. pK_a 8.94 (25°).

▶ LD₅₀ (mus, ori) 95 mg/kg. Exp. reprod. effects. MJ5960000.

Hydrochloride: [125-56-4]. **Methadone**

hydrochloride, USAN. **Physeptone**.

Eptadone. **Metasedin**. **Symoron**

Cryst. Mp 229-230°.

▶ Abuse can lead to habituation or addiction. LD₅₀ (rat, ori) 95 mg/kg. Exp. reprod. and teratogenic effects. MJ6130000.

[1095-90-5]

Easton, N.R. et al, *J.A.C.S.*, 1947, 69, 2941 (synth)

Larsen, A.A. et al, *J.A.C.S.*, 1948, 70, 4194 (synth, resoln)

Hanson, A.W. et al, *Acta Cryst.*, 1958, 11, 724 (cryst struct, abs config)

Bye, E., *Acta Chem. Scand., Ser. B*, 1974, 28, 5 (cryst struct)

Bishara, R.J. et al, *Anal. Profiles Drug Subst.*, 1974, 3, 365; 1980, 9, 601 (rev)

Portoghese, P.S. et al, *J. Med. Chem.*, 1982, 25, 684 (synth)

Buyuktimkin, N. et al, *Arch. Pharm. (Weinheim, Ger.)*, 1984, 317, 653 (resoln)

Duax, W.L. et al, *Tetrahedron*, 1984, 40, 467 (cryst struct)

Säwe, J., *Clin. Pharmacokin.*, 1986, 11, 87 (pharmacokin)

Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, Berlin, 1987, 6228 (synonyms)

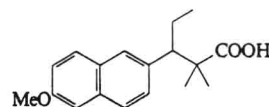
Singh, P. et al, *Acta Cryst. C*, 1989, 45, 1455 (cryst struct)

Martindale, *The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, London, 1993, 1080, 1081.

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DBE100, MDO750, MDO760, MDO775, MDP000, MDP250, MDP500, MDP750.

Methallenestril, INN**M-0-00523**

β -Ethyl-6-methoxy- α,α -dimethyl-2-naphthalenepropanoic acid, 9CI, 8CI. 3-(6-Methoxy-2-naphthyl)-2,2-dimethylpentanoic acid. **Methallenoestril**, BAN. **Cur-men**. **Ercostrol**. **Geklimon**. **Novestrine**. **Vallestril** [517-18-0]



$C_{18}H_{22}O_3$ M 286.3

▶ Exp. reprod. effects. QK0302500.

(–)-form [20756-70-1]

Mp 158-159°. [α]_D –28.5.

(±)-form

Estrogen. Cryst. (MeOH aq.). Mp 139-140°.

[20664-44-2]

Gay, R. et al, *Bull. Soc. Chim. Fr.*, 1955, 955 (synth)

Dubois, J.C. et al, *C. R. Hebd. Seances Acad. Sci.*, 1963, 256, 5596 (resoln)

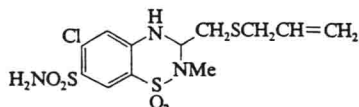
Crenshaw, R.R. et al, *J. Med. Chem.*, 1972, 15, 1179 (pharmacol)

Kuhnert-Brandstaetter, M. et al, *Sci. Pharm.*, 1974, 42, 150 (props, uv)

Martindale, *The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, London, 1993, 1188.

Methalthiazide, USAN M-0-00524

6-Chloro-3,4-dihydro-2-methyl-3-[(2-propenylthio)methyl]-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide, 9CI. 3-[(Allylthio)methyl]-6-chloro-3,4-dihydro-2-methyl-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide, 8CI. P 2530 [5611-64-3]



$C_{12}H_{16}ClN_3O_4S_3$ M 397.9

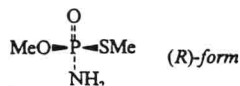
(±)-form

Diuretic, antihypertensive agent. Cryst. (2-propanol). Mp 168.5–170°.

U.K. Pat., 902 658, (1962); CA, 58, 539f (synth, pharmacol)

Methamidophos, BSI M-0-00525

O,S-Dimethyl phosphoramidothioate, 9CI. O,S-Dimethyl amidothiophosphate. Tamaron [10265-92-6]



$C_2H_8NO_2PS$ M 141.1

► Cholinesterase inhibitor. LD₅₀ (rat, orl) 7.5 mg/kg. LD₅₀ (rat, skn) 50 mg/kg. Exp. teratogenic effects. Exp. and human neurotoxic effects. TB4970000.

(R)-form [65960-95-4]

[α]_D +24 (c, 0.5 in CHCl₃).

(±)-form [115182-35-9]

Agricultural systemic insecticide and acaricide. Needles (petrol). Sol. H₂O, EtOH, mod. sol. CHCl₃, C₆H₆, Et₂O.

[65960-97-6]

Lubkowitz, J.A. et al, *J. Agric. Food Chem.*, 1974, 22, 151 (synth, ms, pmr)

Holmstead, R.L. et al, *J. Assoc. Off. Anal. Chem.*, 1974, 57, 1050 (ms)

Hall, C.R. et al, *J.C.S. Perkin 1*, 1979, 1646 (stereochem)

Thompson, C.M. et al, *J. Agric. Food Chem.*, 1982, 30, 282; 1983, 31, 696 (synth, pmr, cmr, tox)

Robinson, C.P. et al, *J. Appl. Toxicol.*, 1982, 2, 217 (tox)

Schneider, P. et al, *J. Prakt. Chem.*, 1982, 324, 1063 (props)

Agrochemicals Handbook, The Royal Society of Chemistry, 1983, A265.

Ripley, B.D. et al, *J. Assoc. Off. Anal. Chem.*, 1983, 66, 1084 (glc)

Miyazaki, A. et al, *J. Agric. Food Chem.*, 1988, 36, 835 (synth, resoln, activity)

Pesticide Manual, 9th edn., 1991, 8090.

Solov'ev, V.N. et al, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1991, 57, 135 (cryst struct)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DTQ400.

Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. et al), Academic Press, 1991, 1090.

Methane, 9CI, 8CI M-0-00526

Marsh gas. Firedamp [74-82-8]

CH₄

CH₄ M 16.0

Widely distributed in nature as product of anaerobic fermentation. The major constit. of natural gas. Illuminating and cooking gas, fuel. Source, via steam reforming, of CO and H₂. Used for industrial prodn. of NH₃, MeOH and other bulk chemicals. Odourless, flammable. Needles when solid. Sol. H₂O, MeOH, most org. solvs. d₄ 0.55 (air = 1.00). Mp –182.6°. Bp –161.4°. pK_a ~ 68–69. Forms a hydrate contg. ca. 6.85 H₂O at 0° under press.

► Extremely flammable, autoignition temp. 537/595°. Forms explosive mixtures with air. An asphyxiant. PA1490000.

Aldrich Library of FT-IR Spectra: Vapor Phase, 3, 1A (ir)

Mathews, J.A., *J.A.C.S.*, 1899, 21, 647 (synth)

Szabo, Z., *J.A.C.S.*, 1950, 72, 3497 (synth)

Fr. Pat., 994 032, (1951); CA, 51, 10836 (synth)

Pasynkiewicz, S. et al, *Annalen*, 1975, 636 (synth)

Breslow, R. et al, *J.A.C.S.*, 1977, 99, 7745 (acidity)

Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, New York, 1978–1984, 12, 901 (rev)

Lin, M. et al, *Nature (London)*, 1994, 368, 613 (synth)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MDQ750.

Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (Snyder, R., Ed.), Elsevier, Volume 1, 1987, 255.

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworth, London and Boston, 1990, 0445.

Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, Cambridge, 1992, 815.

Methanediol, 9CI M-0-00527

Methylene glycol [463-57-0]

CH₂(OH)₂

CH₂O₂ M 48.0

Parent compd. is covalent hydrate of Formaldehyde, F-0-01131 in equilib. with formaldehyde in aq. soln.

Di-Ac: [628-51-3]. Diacetoxymethane.

Methylene diacetate
 $C_6H_8O_4$ M 132.1 Spar. sol. H₂O; misc. EtOH, Et₂O. d₂₀ 1.14. Bp 168–172°, Bp₁₀ 55–60°.

► AI9075000.

Dibenzoyl: [5342-31-4]. *Dibenzoyloxymethane*.

Methylene dibenzoate
 $C_{15}H_{12}O_4$ M 256.2 Cryst. (EtOH). Mp 99°. Bp 220° dec.

Di-Me ether: see Dimethoxymethane, D-0-08409

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1, 948A (nmr)

Aldrich Library of FT-IR Spectra: Vapor Phase, 3, 648D (ir)

Knoevenagel, E., *Annalen*, 1914, 402, 127 (diacetate)

Shaw, J.E. et al, *J.O.C.*, 1974, 39, 1968 (dibenzoate)

Holmberg, K. et al, *Tet. Lett.*, 1975, 2303 (dibenzoate)

Matsuura, H. et al, *Spectrochim. Acta A*, 1980, 36, 321 (Raman)

Le Botlan, D.J. et al, *Anal. Chem.*, 1983, 55, 587 (pmr, cmr)

Williams, I.H. et al, *J.A.C.S.*, 1983, 105, 31.

Methanediphosphonic acid M-0-00528

Methylenebisphosphonic acid, 9CI. Methylenebisphosphonic acid, 8CI. Medronic acid, BAN, USAN, INN

[1984-15-2]

(HO)₂P(O)CH₂P(O)(OH)₂

CH₆O₆P₂ M 176.0

Complexing agent, pharmaceutical aid. Used for prevention of dental caries. Cryst. (2-methyl-2-propanol or AcOH). Mp 201°. pK_{a1} 1.7; pK_{a2} 2.6; pK_{a3} 6.87; pK_{a4} 10.33 (25°), pK_{a1} 1.7; pK_{a2} 2.75; pK_{a3} 7.33; pK_{a4} 10.42 (25°), pK_{a2} 3.05; pK_{a3} 7.35; pK_{a4} 10.96.

Di-Na salt: [25681-89-4]. Amerscan. MDP.

Medronate disodium, USAN

Complex used as bone scanning agent.

Di-NH₄ salt: [108332-58-7].

Cryst.

Tetra-Me ester: [16001-93-7]. Tetramethyl

methylenebisphosphonate

$C_8H_{14}O_6P_2$ M 232.1 Liq. Bp_{0.05} 87–90°. n_D²⁰ 1.4523.

Tetra-Et ester: [1660-94-2]. Tetraethyl

methylenebisphosphonate

$C_9H_{22}O_6P_2$ M 288.2 Liq. Bp₆ 160–165°, Bp_{0.8} 126–130°. n_D²⁰ 1.4412 (1.4300).

► SZ9150000.

Tetrabutyl ester: [6997-56-4]. Tetrabutyl

methylenebisphosphonate

$C_{17}H_{38}O_6P_2$ M 400.4 Liq. d₄²⁵ 1.04. Bp_{0.0005} 150–155°. n_D²⁰ 1.4455.

Tetrakis(2-propenyl) ester: [25091-05-8].

Tetraallyl methylenediphosphonate

$C_{13}H_{22}O_6P_2$ M 336.2 Liq. d₄²⁰ 1.13. Bp_{0.1} 142°. n_D²⁰ 1.4675.

► May dec. violently on attempted distn.

Tetraisopropyl ester: [1660-95-3]. Tetrakis(1-

methylethyl) methylenebisphosphonate.

Tetraisopropyl methylenediphosphonate

$C_{13}H_{26}O_6P_2$ M 344.3 Liq. Bp_{0.1} 96–100°. n_D²⁰ 1.4317.

P,P-Di-Ph ester: P,P-Diphenyl

methylenebisphosphonate

$C_{13}H_{14}O_6P_2$ M 328.1 Solid. Mp 146–151°.

P,P'-Di-Ph ester: [108925-83-3]. P,P'-

Diphenyl methylenebisphosphonate

$C_{13}H_{14}O_6P_2$ M 328.1 Solid. Mp 177–179°.

Tri-Ph ester: Triphenyl

methylenebisphosphonate

$C_{19}H_{18}O_6P_2$ M 404.2 Liq. Bp_{0.03} 165°.

Tetra-Ph ester: [84441-53-2]. Tetraphenyl

methylenebisphosphonate

$C_{25}H_{22}O_6P_2$ M 480.3 Needles (Et₂O). Mp 81–82°.

Tetrafluoride: see Methylenebis[phosphonic difluoride], M-0-02017

Tetrachloride: see Methylenebis[phosphonic dichloride], M-0-02016

Tetraamide: see P,P'-Methylenebis[phosphonic diamide], M-0-02015

[126589-89-7]

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Aldrich Library of FT-IR Spectra, 1st edn., 1, 915A (ir)