Dictionary of Organic Compounds

SIXTH EDITION

VOLUME TWO

Bromethalin–Dib

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Each volume will contain about 2,000 new and revised entries derived from the primary literature of the preceding year, and will provide a complete updating service for all organic chemistry. Cumulative indexes will appear in supplements as space permits.

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London SE1 8HN

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Treat all chemical substances as if they have dangerous properties.

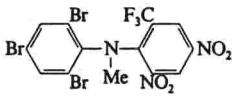
The publisher makes no representation, express or implied, with regard to the accuracy of the information contained in this Dictionary, and cannot accept any legal responsibility or liability for any errors or omissions that may be made.

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.

Bromethalin, BSI, ISO, ANSI **B-0-03702**

N-Methyl-2,4-dinitro-N-(2,4,6-tribromophenyl)-6-(trifluoromethyl) benzenamine, 9CI. α,α,α-Trifluoro-N-methyl-4,6-dinitro-N-(2,4,6-tribromophenyl)-o-toluidine. 2,4,6-Tribromo-N-methyl-2',4'-dinitro-6'-(trifluoromethyl)diphenylamine. Vengeance

[63333-35-7]



$C_{14}H_7Br_3F_3N_3O_4$ M 577.9

Rodenticide. Oxidative phosphorylation uncoupler. Pale yellow cryst. Mp 150-151°.

▶ LD_{50} (rat, orl) 2 mg/kg. CY0383000.

U.S. Pat., 4 187 318, (1980); *CA*, **92**, 215040y (*synth, activity*)

Dreikorn, B.A. *et al, Acta Chem. Scand.*, 1984, **255**, 45 (*rev, props*)

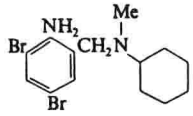
Van Lier, B.L. *et al, Fundam. Appl. Toxicol.*, 1988, **11**, 664 (*metab, tox*)

Pesticide Manual, 9th edn., 1991, 96.

Bromhexine, BAN, INN **B-0-03704**

2-Amino-3,5-dibromo-N-cyclohexyl-N-methylbenzenemethanamine, 9CI. 3,5-Dibromo-N$^{\alpha}$-cyclohexyl-N$^{\alpha}$-methyltoluene-α,2-diamine, 8CI

[3572-43-8]



$C_{14}H_{20}Br_2N_2$ M 376.1

Bronchial mucolytic and expectorant. Used mainly as hydrochloride.

Hydrochloride: [611-75-6]. ***Bromhexine hydrochloride*, USAN, JAN.** *Brozime. Bisolvon. Bromexina. Many other names*

Insol. Me_2CO, $CHCl_3$. Mp 237-238° dec.

▶ LD_{50} (rat, orl) 6 g/kg. XS9950000.

Keck, J., *Annalen*, 1963, **662**, 171 (*synth*)

Engelhorn, R. *et al, Arzneim.-Forsch.*, 1963, **13**, 474 (*pharmacol*)

Boyd, E.M. *et al, Arch. Int. Pharmacodyn. Ther.*, 1966, **163**, 284 (*props, tox*)

Jaunch, R. *et al, Arzneim.-Forsch.*, 1975, **25**, 1954 (*metab*)

Shimizu, N. *et al, Acta Cryst. C*, 1983, **39**, 891; 1984, **40**, 902 (*cryst struct*)

Koo, C.H. *et al, Arch. Pharmacal. Res.*, 1984, **7**, 115 (*struct*)

Yang, T.C., *CA*, 1984, **101**, 191225 (*synth*)

Eur. Pat., 130 224, (1985); *CA*, **103**, 37181 (*synth*)

Nardi, D. *et al, Farmaco, Ed. Sci.*, 1985, **40**, 108 (*pharmacol*)

Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, Berlin, 1987, 3253 (*synonyms*)

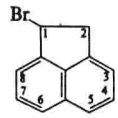
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 744.

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BMO325.

1-Bromoacenaphthene **B-0-03705**

1-Bromo-1,2-dihydroacenaphthylene, 9CI. 7-Bromoacenaphthene (obsol.)

[24171-73-1]



$C_{12}H_9Br$ M 233.1

(±)-form

Yellowish leaflets. Mp 70.5-71.5°. Unstable.

Bachmann, W.E. *et al, J.A.C.S.*, 1941, **63**, 204 (*synth*)

Craniadès, P. *et al, Bull. Soc. Chim. Fr.*, 1954, 719 (*synth*)

Dewar, M.J.S. *et al, J.A.C.S.*, 1963, **85**, 2704 (*pmr*)

Petrenko, G.P. *et al, Zh. Org. Khim.*, 1969, **5**, 2023 (*synth*)

Rice, J.E. *et al, J.O.C.*, 1990, **55**, 5490 (*synth, pmr, cmr*)

3-Bromoacenaphthene **B-0-03706**

3-Bromo-1,2-dihydroacenaphthylene, 9CI. 2-Bromoacenaphthene (obsol.)

[5209-31-4]

$C_{12}H_9Br$ M 233.1

Needles (MeOH). Mp 78°.

Morgan, G.T. *et al, J. Soc. Chem. Ind., London*, 1930, **49**, 413T (*synth*)

Vorozhtsov, N.N. *et al, CA*, 1960, **54**, 445 (*synth, uv*)

Deady, L.W. *et al, Appl. Spectrosc.*, 1974, **28**, 552 (*ir*)

Red'kin, Yu.P. *et al, Opt. Spektrosk.*, 1975, **38**, 60, 283 (*uv*)

4-Bromoacenaphthene **B-0-03707**

4-Bromo-1,2-dihydroacenaphthylene, 9CI

[4657-98-1]

$C_{12}H_9Br$ M 233.1

Needles by subl. Mp 65-66°.

Vorozhtzov, N.N. *et al, CA*, 1960, **54**, 445 (*synth, uv*)

Topsom, R.D. *et al, Spectrochim. Acta*, 1963, **19**, 1859 (*ir*)

Cava, P. *et al, Tetrahedron*, 1965, **21**, 3059 (*synth*)

5-Bromoacenaphthene **B-0-03708**

5-Bromo-1,2-dihydroacenaphthylene, 9CI. 4-Bromoacenaphthene (obsol.). 3-Bromoacenaphthene (obsol.)

[2051-98-1]

$C_{12}H_9Br$ M 233.1

Plates or light-yellow needles (EtOH). Mp 53-54°. Bp 335-336°, Bp_{19} 185-190°.

Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1029D (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 961B (*ir*)

Aldrich Library of NMR Spectra, 2nd edn., **1**, 828D (*nmr*)

Crompton, H. *et al, J.C.S.*, 1912, 958 (*synth*)

Buu-Hoï, Ng.Ph., *Annalen*, 1944, **556**, 1 (*synth*)

Carpignaro, R., *Gazz. Chim. Ital.*, 1956, **86**, 132 (*uv*)

Ross, S.D. *et al, J.A.C.S.*, 1958, **80**, 4327 (*synth*)

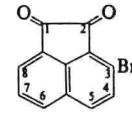
Deady, L.W. *et al, Appl. Spectrosc.*, 1974, **28**, 552 (*ir*)

Red'kin, Yu.P. *et al, Opt. Spektrosk.*, 1975, **38**, 60, 283 (*uv*)

3-Bromoacenaphthenequinone **B-0-03709**

3-Bromo-1,2-acenaphthylenedione, 9CI. 2-Bromoacenaphthenequinone (obsol.)

[21170-55-8]



$C_{12}H_5BrO_2$ M 261.0

Because of differing numbering systems some early refs. are unclear as to which isomer was prepared in this series. Only recent refs. have been quoted.

Petrenko, G.P. *et al, Zh. Org. Khim.*, 1973, **9**, 2313 (*synth*)

4-Bromoacenaphthenequinone **B-0-03710**

4-Bromo-1,2-acenaphthylenedione, 9CI. 5-Bromoacenaphthenequinone (obsol.)

[43017-97-6]

$C_{12}H_5BrO_2$ M 261.0

See note under 3-Bromoacenaphthenequinone, B-0-03709. Yellow needles (AcOH). Mp 219-220°.

Krivoshapko, N.G. *et al, Ukr. Khim. Zh.* (*Russ. edn.*), 1973, **39**, 802 (*synth*)

5-Bromoacenaphthenequinone **B-0-03711**

5-Bromo-1,2-acenaphthylenedione, 9CI. 3-Bromoacenaphthenequinone (obsol.). 4-Bromoacenaphthenequinone (obsol.)

[26254-35-3]

$C_{12}H_5BrO_2$ M 261.0

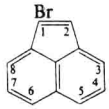
See note under 3-Bromoacenaphthenequinone, B-0-03709. Pale-yellow or orange needles (EtOH or AcOH). Mp 231-232°, Mp 246°.

Dewhurst, F. *et al, J.C.S.(C)*, 1970, 1737 (*synth*)

Petrenko, G.P. *et al, Zh. Org. Khim.*, 1973, **9**, 786, 2313 (*synth*)

1-Bromoacenaphthylene B-0-03712

[54736-49-1]



$C_{12}H_7Br$ M 231.0
Oil.

Picrate: Yellow needles (EtOH). Mp 145-146.5°.

Greene, F.D. *et al, J.A.C.S.*, 1957, **79**, 1416 (*synth*)
Krishnan, S. *et al, Environ. Sci. Technol.*, 1979, **13**, 1532 (*synth, ms*)

3-Bromoacenaphthylene B-0-03713

[20371-51-1]

$C_{12}H_7Br$ M 231.0
Yellow cryst. (MeOH). Mp 62.5-63.5°.

Petrenko, G.P. *et al, J. Org. Chem. USSR (Engl. Transl.)*, 1968, **4**, 1233; 1969, **5**, 719 (*synth, uv*)

4-Bromoacenaphthylene B-0-03714

[23921-32-6]

$C_{12}H_7Br$ M 231.0
Oil.

Picrate: Yellow cryst. (C_6H_6). Mp 143.5-144.5°.

Petrenko, G.P., *J. Org. Chem. USSR (Engl. Transl.)*, 1969, **5**, 719 (*synth, uv*)

5-Bromoacenaphthylene B-0-03715

[7267-03-0]

$C_{12}H_7Br$ M 231.0
Yellow plates (butanol). Mp 59-60°.

Petrenko, G.P. *et al, J. Org. Chem. USSR (Engl. Transl.)*, 1966, **2**, 724; 1969, **5**, 719 (*synth, uv*)
Mitchell, R.H. *et al, Can. J. Chem.*, 1992, **70**, 1015 (*synth, pmr, cmr*)

Bromoacetaldehyde B-0-03716

Bromoethanal

[17157-48-1]

$BrCH_2CHO$

C_2H_3BrO M 122.9
Bp 107-112°.

▶ AB2190000.

Semicarbazone: Cryst. (EtOH). Mp 128° dec.
2,4-Dinitrophenylhydrazone: Orange cryst. Mp 155-156°.
Di-Me acetal: [7252-83-7]. *2-Bromo-1,1-dimethoxyethane*
$C_4H_9BrO_2$ M 169.0 d_4^{20} 1.430. Bp_{14} 48-49°.
Di-Et acetal: [2032-35-1]. *2-Bromo-1,1-diethoxymethane*
$C_6H_{13}BrO_2$ M 197.0 d 1.31. Bp_{18} 66-67°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **1**, 360A, 360C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 221A, 221D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 291B, 291D (*ir*)
Hibbert, H. *et al, J.A.C.S.*, 1923, **45**, 743 (*synth*)
Stepanow, A. *et al, Ber.*, 1925, **58**, 1718 (*synth*)
Bedoukian, P.Z., *J.A.C.S.*, 1944, **66**, 651.
Wizinger, R. *et al, Helv. Chim. Acta*, 1947, **30**, 189 (*synth*)
Bose, J.L. *et al, J.C.S.*, 1959, 3314.
Ross, A. *et al, J.O.C.*, 1961, **26**, 579.
Kraus, G.A. *et al, J.O.C.*, 1983, **48**, 2111 (*synth, use*)
Liebeskind, L.S. *et al, J.O.C.*, 1989, **54**, 1435 (*acetal*)
Jachak, M. *et al, Org. Prep. Proced. Int.*, 1993, **25**, 469 (*synth, bibl*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BMR000.

N-Bromoacetamide B-0-03717

Acetobromoamide†

[79-15-2]

$H_3CCONHBr$

C_2H_4BrNO M 137.9
Brominating and oxidising agent. Cryst. ($CHCl_3$/hexane). Sol. hot H_2O. Mp 108°. Light sensitive.

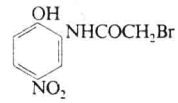
▶ Can dec. hazardously when hot. Eye, skin and respiratory tract irritant.

Org. Synth., Coll. Vol., 4, 1963, 104 (*synth*)
Dubey, R.J., *Acta Cryst. B*, 1971, **27**, 23 (*cryst struct*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 61.
Fujisaki, S. *et al, Bull. Chem. Soc. Jpn.*, 1993, **66**, 2426 (*synth*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th edn., Van Nostrand Reinhold, 1979, 432.
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworth, London and Boston, 1990, 0736.
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, Cambridge, 1992, 162.

2-(Bromoacetamido)-4-nitrophenol B-0-03718

2-Bromo-N-(2-hydroxy-5-nitrophenyl) acetamide, 9CI. 2-Bromo-2'-hydroxy-5'-nitroacetanilide. Koshland's reagent III

[3947-58-8]



$C_8H_7BrN_2O_4$ M 275.0
Reacts with chymotrypsin to produce a reporter-labelled protein. Cryst. (EtOH aq.). Sol. MeOH, Me_2CO, C_6H_6. Mp 215-220° dec.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 1371A (*nmr*)
Aldrich Library of Infrared Spectra, 3rd edn., 1070G (*ir*)
Burr, M. *et al, J.A.C.S.*, 1967, **89**, 5945 (*synth, use*)
Horton, H.R. *et al, Methods Enzymol.*, 1967, **11**, 856 (*use*)
Lewis, S.D. *et al, Biochemistry*, 1974, **13**, 690 (*use*)
Sams, C.F. *et al, J. Biol. Chem.*, 1977, **252**, 3153 (*use*)

Bromoacetic acid B-0-03719

Bromoethanoic acid

[79-08-3]

$BrCH_2COOH$

$C_2H_3BrO_2$ M 138.9
Sol. H_2O, EtOH. Mp 50°. Bp 208°. pK_a 2.86 (25°).

▶ Irritant and corrosive to skin and mucous membranes. Skin effects may be delayed. LD_{50} (mus, orl) 100 mg/kg. AF5950000.

Me ester: [96-32-2].
$C_3H_5BrO_2$ M 152.9 Bp 144° dec.
▶ Strong lachrymator. AF6300000.

Et ester: [105-36-2].
$C_4H_7BrO_2$ M 167.0 Synthetic reagent. d 1.51. Bp 159°.
▶ Eye and skin irritant. AF6000000.

2-Propenyl ester: [40630-84-0].
$C_5H_7BrO_2$ M 179.0 Bp_{10} 73°.

tert-*Butyl ester:* [5292-43-3].
$C_6H_{11}BrO_2$ M 195.0 Bp_{10} 50°. n_D^{20} 1.4450.

Benzyl ester: [5437-45-6].
$C_9H_9BrO_2$ M 229.0 Bp_{22} 166-170°. n_D^{20} 1.5440.
▶ AF5957215.

Ph ester: [620-72-4].
$C_8H_7BrO_2$ M 215.0 Mp 32°. Bp_{20} 140°.

Chloride: [22118-09-8].
C_2H_2BrClO M 157.3 Bp 133-135°.

Bromide: [598-21-0].
$C_2H_2Br_2O$ M 201.8 d_{25}^{25} 2.317. Bp 150°.

Amide: [683-57-8]. *Bromoacetamide. Acetobromoamide*†
C_2H_4BrNO M 137.9 Sol. H_2O, EtOH. Mp 91° (85-87°).
▶ AB4587000.

Nitrile: [590-17-0]. *Bromoacetonitrile. Bromocyanomethane*
C_2H_2BrN M 119.9 Bp_{752} 150-151°.
▶ AL7970000.

Anhydride: [13094-51-4].
$C_4H_4Br_2O_3$ M 259.8 Mp 41-42°. Bp 230-232° dec.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **1**, 790C, 1007B, 1009B, 1013B, 1222C, 1366A; **2**, 1202B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 508B, 508D, 651A, 651B, 652B, 724A, 848B; **2**, 277B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 700C, 700D, 702B, 766A, 1336D (*ir*)
Steinkopf, W., *Ber.*, 1912, **45**, 3136 (*anhydride*)
Ward, C.F., *J.C.S.*, 1922, **121**, 1161 (*synth*)
Natelson, S. *et al, J.A.C.S.*, 1939, **61**, 970 (*synth*)
Smissman, E.E., *J.A.C.S.*, 1954, **76**, 5805 (*anhydride*)
Org. Synth., Coll. Vol., 3, 1955, 381 (*synth*)
Ray, W.J. *et al, Appl. Spectrosc.*, 1979, **33**, 492 (*uv, ir*)
Dillon, K.B. *et al, J. Magn. Reson.*, 1980, **39**, 499 (*pmr*)
Field, L.D. *et al, Org. Magn. Reson.*, 1984, **22**, 221 (*cmr*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BMR750, EGV000, MHR250.
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, Cambridge, 1992, 163.

2-Bromoacetophenone B-0-03720

2-Bromo-1-phenylethanone, 9CI. Phenacyl bromide. Bromomethyl phenyl ketone

[70-11-1]

$PhCOCH_2Br$

C_8H_7BrO M 199.0
Derivatisation reagent for carboxylic acids for hplc anal. Anal. reagent for thioureas and thiosemicarbazones. Prisms (EtOH aq.). Mp 51°. Bp_{18} 135°.

▶ Corrosive and irritating to all tissues. AM5978400.

(E)-*Oxime:* [17082-14-3]. anti-*Oxime*
C_8H_8BrNO M 214.0 Mp 114-114.5°.

(Z)-*Oxime:* [17082-13-2]. syn-*Oxime*
Mp 97°.

Semicarbazone: Mp 146°.

2,4-Dinitrophenylhydrazone: [4880-96-0]. Yellow-orange cryst. Mp 220°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 825A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 20C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1240C (*ir*)
Org. Synth., Coll. Vol., 2, 1943, 480 (*synth*)
Yanovskaya, L. *et al*, *Zh. Obshch. Khim.*, 1952, **22**, 1598; *CA*, **47**, 9258 (*synth*)
Gupta, M. *et al*, *Acta Cryst. B*, 1971, **27**, 1649 (*cryst struct*)
Kaiser, E. *et al*, *J.A.C.S.*, 1972, **94**, 9274 (*nmr, uv, oxime*)
Wetherington, J. *et al*, *Acta Cryst. B*, 1973, **29**, 1520 (*cryst struct, oxime*)
Borch, R.F., *Anal. Chem.*, 1975, **47**, 2437 (*use*)
Pannell, K. *et al*, *Org. Mass Spectrom.*, 1975, **10**, 550 (*ms*)
Khanna, N. *et al*, *Talanta*, 1978, **25**, 591 (*use*)
Talegaonkar, J. *et al*, *Talanta*, 1982, **29**, 327 (*use*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th edn., Van Nostrand Reinhold, 1979, 432.
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, Cambridge, 1992, 991.

2′-Bromoacetophenone B-0-03721

1-(2-Bromophenyl)ethanone, 9CI. o-*Bromophenyl methyl ketone*

[2142-69-0]

C_8H_7BrO M 199.0
Pale-yellow liq. Bp_{10} 112°.

Semicarbazone: Prisms (EtOH). Mp 177°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 829A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 23D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1242C (*ir*)
Elson, L. *et al*, *J.C.S.*, 1930, 1128 (*synth*)
Smith, W. *et al*, *J.A.C.S.*, 1972, **94**, 1959 (*nmr*)
Kreuger, P. *et al*, *Can. J. Chem.*, 1973, **51**, 1363 (*ir*)
Tomasik, P. *et al*, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1974, **22**, 1065; *CA*, **82**, 124540 (*uv*)

3′-Bromoacetophenone B-0-03722

1-(3-Bromophenyl)ethanone, 9CI. m-*Bromophenyl methyl ketone*

[2142-63-4]

C_8H_7BrO M 199.0
Liq. Mp 7-8°. Bp_{16} 131°. pK_{a1} −6.90 (25°, H_2SO_4 aq.).

Semicarbazone: Needles (EtOH). Mp 232-233°, Mp 238° dec.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 830B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 24C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1243B (*ir*)
Elson, L. *et al*, *J.C.S.*, 1930, 1128 (*synth*)
Hinton, J. *et al*, *Org. Magn. Reson.*, 1972, **4**, 353 (*cmr*)
Twine, C. *et al*, *J.O.C.*, 1974, **39**, 1290 (*ir, uv, ms*)
Eizember, R. *et al*, *Org. Prep. Proced. Int.*, 1974, **6**, 251; *CA*, **82**, 97788 (*synth*)

4′-Bromoacetophenone B-0-03723

1-(4-Bromophenyl)ethanone, 9CI. p-*Bromophenyl methyl ketone*

[99-90-1]

C_8H_7BrO M 199.0
Leaflets. Mp 51°. Bp_{736} 255.5°, Bp_7 117°. pK_{a1} −6.52 (H_2SO_4 aq.).

Oxime: [5798-71-0].
C_8H_8BrNO M 214.0 Mp 128-129°.

Hydrazone:
$C_8H_9BrN_2$ M 213.0 Mp 164°.

2,4-Dinitrophenylhydrazone: [2772-50-1]. Mp 235-237°.

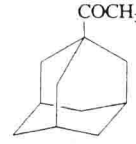
[59862-55-4, 73744-33-9]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 832C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 30D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1251B (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 109 (*synth*)
Hinton, J. *et al*, *Org. Magn. Reson.*, 1972, **4**, 353 (*cmr*)

1-(Bromoacetyl)adamantane B-0-03724

1-Adamantyl bromomethyl ketone, 8CI. 2-Bromo-1-tricyclo[3.3.1.1^{3,7}]dec-1-ylethanone, 9CI

[5122-82-7]



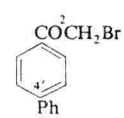
$C_{12}H_{17}BrO$ M 257.1
Powder (MeOH). Mp 78-79°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **1**, 666A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 430B (*ir*)
Stetter, H. *et al*, *Chem. Ber.*, 1960, **93**, 2054 (*synth*)
Sasaki, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1969, **42**, 1617 (*synth, ir*)
Stepanov, F.N. *et al*, *J. Org. Chem. USSR (Engl. Transl.)*, 1970, **6**, 50 (*synth*)

4-(Bromoacetyl)biphenyl B-0-03725

1-[(1,1′-Biphenyl)-4-yl]-2-bromoethanone, 9CI. p-*Phenylphenacyl bromide. 2-Bromo-4′-phenylacetophenone, 8CI*

[135-73-9]



$C_{14}H_{11}BrO$ M 275.1
Reagent used for identifying acids. Mp 125.5°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 827A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 22B (*ir*)
Drake, N.L. *et al*, *J.A.C.S.*, 1930, **52**, 3715 (*synth*)
Buu-Hoï, Ng.Ph. *et al*, *Bull. Soc. Chim. Fr.*, 1950, 489 (*synth*)
Jart, A., *CA*, 1965, **63**, 14654 (*ir*)
Umeh, E.O., *J. Chromatogr.*, 1971, **56**, 29 (*use*)

Bromoacetylene B-0-03726

Bromoethyne

[593-61-3]

$CH{\equiv}CBr$

C_2HBr M 104.9
Gas which polymerises in light. Sol. H_2O, dil. HNO_3. Bp 4.7° (−2°).

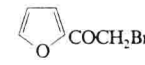
▶ Unstable, spontaneously flammable, may explode on contact with air.

Nef, J.U., *Annalen*, 1897, **298**, 357 (*synth*)
Hofmann, K.A. *et al*, *Ber.*, 1909, **42**, 4235 (*synth*)
Bashford, L.A. *et al*, *J.C.S.*, 1938, 1358 (*synth*)
Haink, H.J. *et al*, *Helv. Chim. Acta*, 1970, **53**, 1073 (*pe*)
Kloster-Jensen, E. *et al*, *Helv. Chim. Acta*, 1970, **53**, 2109 (*ms*)
Kloster-Jensen, E. *et al*, *Tet. Lett.*, 1972, 4023 (*pmr*)
Hucknall, D.J. *et al*, *Spectrosc. Lett.*, 1974, **7**, 381 (*ir*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BMS500.
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworth, London and Boston, 1990, 0617.
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, Cambridge, 1992, 165.

2-(Bromoacetyl)furan B-0-03727

2-Bromo-1-(2-furanyl)ethanone

[15109-94-1]



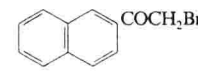
$C_6H_5BrO_2$ M 189.0
Cryst. (petrol). Mp 34°. $Bp_{0.15}$ 72-74°.

Arcoria, A. *et al*, *J. Het. Chem.*, 1975, **12**, 215.
Dubac, J. *et al*, *Synth. Commun.*, 1991, **21**, 11 (*synth, pmr*)

2-(Bromoacetyl)naphthalene B-0-03728

2-Bromo-1-(2-naphthalenyl)-1-ethanone, 9CI. 2-Bromo-2′-acetonaphthone, 8CI. 2-Naphthacyl bromide

[613-54-7]



$C_{12}H_9BrO$ M 249.1
Reagent for esterification of fatty acids for hplc anal. Needles (EtOH). Mp 81-82°.

Picrate: Needles (EtOH). Mp 93°.
Oxime: Cryst. (MeOH). Mp 174°.

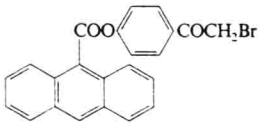
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 827B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 22D (*ir*)

Radcliffe, C.B. *et al*, *J.C.S.*, 1931, 2293 (*synth*)
Immediata, T. *et al*, *J.O.C.*, 1940, **5**, 512 (*synth*)
Cooper, M.J. *et al*, *Anal. Chem.*, 1974, **46**, 1849 (*use*)
Prasad, K.N., *Indian J. Pure Appl. Phys.*, 1982, **20**, 412; *CA*, **97**, 47699c (*cryst struct*)
Kihara, K. *et al*, *Bunseki Kagaku (Jpn. Anal.)*, 1984, **33**, 647; *CA*, **102**, 1476249q (*use*)

4-(Bromoacetyl)phenyl 9-anthracenecarboxylate, 9CI B-0-03729

4-(9-Anthroyloxy)phenacyl bromide. Panacyl bromide

[94345-04-7]

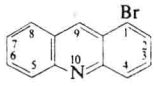


$C_{23}H_{15}BrO_3$ M 419.2
Used as hplc derivatisation reagent for prostaglandins. Deep yellow cryst. Mp 173.3-173.6°.

Cox, J.W. *et al*, *Anal. Chem.*, 1984, **56**, 1866 (*use*)
Salari, H. *et al*, *Anal. Biochem.*, 1987, **165**, 220 (*synth, use*)

1-Bromoacridine B-0-03730

[4357-63-5]



$C_{13}H_8BrN$ M 258.1
Yellow needles (petrol). Mp 110-111°. pK_a 3.05 (50% EtOH).

Chandler, G.S. *et al*, *Aust. J. Chem.*, 1965, **18**, 108.
Graboyes, H. *et al*, *J. Het. Chem.*, 1975, **12**, 1225.

2-Bromoacridine B-0-03731

[4357-58-8]

$C_{13}H_8BrN$ M 258.1
Pale-yellow needles (petrol). Mp 175-175.5°. pK_a 2.28 (50% EtOH).

Acheson, R.M. *et al*, *J.C.S.*, 1954, 4142.
Chandler, G.S. *et al*, *Aust. J. Chem.*, 1965, **18**, 108.
Graboyes, H. *et al*, *J. Het. Chem.*, 1975, **12**, 1225.

3-Bromoacridine B-0-03732

[4357-62-4]

$C_{13}H_8BrN$ M 258.1
Pale-yellow plates (petrol). Mp 137-138°. pK_a 3.08 (50% EtOH).

Chandler, G.S. *et al*, *Aust. J. Chem.*, 1965, **18**, 108.
Graboyes, H. *et al*, *J. Het. Chem.*, 1975, **12**, 1225.

4-Bromoacridine B-0-03733

[4357-61-3]

$C_{13}H_8BrN$ M 258.1
Cryst. (petrol). Mp 107-108°. pK_a 2.02 (50% EtOH).

Chandler, G.S. *et al*, *Aust. J. Chem.*, 1965, **18**, 108.
Graboyes, H. *et al*, *J. Het. Chem.*, 1975, **12**, 1225.

9-Bromoacridine B-0-03734

ms-*Bromoacridine*

[4357-57-7]

$C_{13}H_8BrN$ M 258.1
Needles (EtOH/NH_3 aq.). Mp 116°.

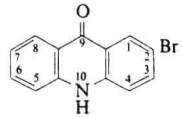
N-*Oxide:* [10228-96-3].
$C_{13}H_8BrNO$ M 274.1 Yellow needles (MeCN). Mp 174°.

Acheson, R.M. *et al*, *J.C.S.*, 1960, 3367.

2-Bromo-9(10*H*)-acridinone, 9CI B-0-03735

2-Bromoacridone

[7497-54-3]



$C_{13}H_8BrNO$ M 274.1
Brownish-yellow needles with very high Mp.

Lehmstedt, K., *Ber.*, 1932, **65**, 839.
Badger, G.M. *et al*, *J.C.S.*, 1952, 1874.

3-Bromo-9(10*H*)-acridinone, 9CI B-0-03736

[1140-92-7]

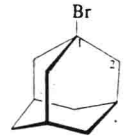
$C_{13}H_8BrNO$ M 274.1
Pale-yellow needles (AcOH). Mp >360°.

Ullman, F., *Annalen*, 1907, **355**, 341.

1-Bromoadamantane B-0-03737

1-Bromotricyclo[3.3.1.1^{3,7}]decane, 9CI

[768-90-1]



$C_{10}H_{15}Br$ M 215.1
Mp 116-118°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **1**, 157C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 105C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 148D (*ir*)
Clive, D.L. *et al*, *Chem. Comm.*, 1971, 1112 (*synth*)
Osawa, E. *et al*, *Tet. Lett.*, 1974, 115 (*synth*)
Grob, C.A. *et al*, *Helv. Chim. Acta*, 1988, **71**, 1508 (*synth*)

2-Bromoadamantane B-0-03738

2-Bromotricyclo[3.3.1.1^{3,7}]decane, 9CI

[7314-85-4]

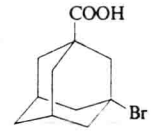
$C_{10}H_{15}Br$ M 215.1
Cryst. (EtOH). Mp 138-140°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **1**, 158A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 105D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 149A (*ir*)
Hoek, W. *et al*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1966, **85**, 1045 (*synth*)
Olah, G.A. *et al*, *Synthesis*, 1974, 653 (*synth*)
Olah, G.A. *et al*, *J.O.C.*, 1979, **44**, 3872 (*synth*)

3-Bromo-1-adamantanecarboxylic acid B-0-03739

3-Bromotricyclo[3.3.1.1^{3,7}]decane-1-carboxylic acid, 9CI

[21816-08-0]



$C_{11}H_{15}BrO_2$ M 259.1
Cryst. (cyclohexane). Mp 146.5°. pK_a 6.28 (50% EtOH aq., 25°).

▶ AU4452500.

Me ester: [27983-08-0].
$C_{12}H_{17}BrO_2$ M 273.1 Cryst. (petrol at −40°). Mp 32°.

Stetter, H. *et al*, *Chem. Ber.*, 1960, **93**, 1366; 1962, **95**, 667 (*synth*)
Bayal, M.L. *et al*, *Zh. Org. Khim.*, 1973, **99**, 290, 291; *J. Org. Chem. USSR (Engl. Transl.)*, 1973, **9**, 290.

2-Bromoaniline B-0-03740

2-Bromobenzenamine, 9CI

[615-36-1]

C_6H_6BrN M 172.0
Fp 28.7°, Mp 32°. Bp_{48-53} 138-141°. pK_a 2.48 (no solv. given).

▶ Fl.p. >66°.

Picrate: [54575-26-7].
Mp 128.5°.
N-*Formyl:* [10113-38-9].
C_7H_6BrNO M 200.0 Cryst. Mp 87°.
N-*Ac:* [614-76-6].
C_8H_8BrNO M 214.0 Cryst. Mp 99°.
N-*Benzoyl:* [70787-27-8].
$C_{13}H_{10}BrNO$ M 276.1 Mp 116°.
▶ CV2430520.
N-*Me:* [6832-87-7].
C_7H_8BrN M 186.0 Bp_{14} 117°.
N-*Di-Me:* [698-00-0].
$C_8H_{10}BrN$ M 200.0 Liq. d_{25}^{25} 1.39. Bp_{14} 107-108°.
N-*Di-Me, picrate:* Mp 150-151°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 462B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1195A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1114D (*ir*)
Hewitt, J.H. *et al*, *J.C.S.*, 1901, 160 (*synth*)
v. Auwers, K., *Ber.*, 1907, **40**, 2524 (*deriv*)
West, R.W., *J.C.S.*, 1925, 494 (*synth*)
Roberts, J.D. *et al*, *Org. Magn. Reson.*, 1974, **6**, 636 (*nmr*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th edn., Van Nostrand Reinhold, 1979, 432.

3-Bromoaniline B-0-03741

3-Bromobenzenamine, 9CI

[591-19-5]

C_6H_6BrN M 172.0
$d_4^{20.4}$ 1.58. Fp 16.7°, Mp 18.5°. Bp_{12} 130°. pK_{a1} 3.53 (25°).

▶ Fl. p. >66°. CX9855300.

Picrate: Mp 180°.

N-*Ac:* [621-38-5].
C_8H_8BrNO M 214.0 Mp 87.5°.

N-*Benzoyl:* [10286-85-8].
$C_{13}H_{10}BrNO$ M 276.1 Mp 120°.
▶ CV2430525.

N-*Di-Me:* [16518-62-0].
$C_8H_{10}BrN$ M 200.0 Mp 11°. Bp 259°, Bp_2 100-104°.

N-*Di-Et:* [53142-19-1].
$C_{10}H_{14}BrN$ M 228.1 Bp_{9-10} 140-142°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 468B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1199A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1118D (*ir*)
Holleman, A.F., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1906, **25**, 186 (*synth*)
Miyajima, G. *et al*, *Chem. Pharm. Bull.*, 1971, **19**, 2301 (*cmr*)
Roberts, J.D. *et al*, *Org. Magn. Reson.*, 1974, **6**, 636 (*nmr*)

4-Bromoaniline B-0-03742

4-Bromobenzenamine, 9CI

[106-40-1]

C_6H_6BrN M 172.0
Mp 66°. pK_{a1} 3.94 (25°).

▶ LD_{50} (rat, orl) 456 mg/kg. BW9280000.

N-*Formyl:* [2617-78-9]. N-(*4-Bromophenyl*) *formamide, 9CI*
C_7H_6BrNO M 200.0 Mp 119°.
▶ LQ4663000.

N-*Ac:* [103-88-8].
C_8H_8BrNO M 214.0 Mp 168°.
▶ AD9625000.

N-*Benzoyl:* [7702-38-7].
$C_{13}H_{10}BrNO$ M 276.1 Cryst. (EtOH). Mp 202°.
▶ CV2430530.

N-*Me:* [6911-87-1].
C_7H_8BrN M 186.0 Bp 259-260°, Bp_{14} 137-138°.

N,N-*Di-Me:* [586-77-6].
$C_8H_{10}BrN$ M 200.0 Cryst. Mp 55°. Bp 264°.
▶ Can explode during distillation in vacuo. Irritant. BW9300000.

N-*Et:* [68254-64-8].
$C_8H_{10}BrN$ M 200.0 Mp 12°. Bp_{20} 143-147°.

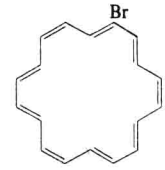
N,N-*Di-Et:* [2052-06-4].
$C_{10}H_{14}BrN$ M 228.1 Cryst. (EtOH). Mp 33°. Bp 270°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 482A, 482B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1207C, 1261D; **2**, 357D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1127A, 1127B (*ir*)
Vecchiotti, L., *Gazz. Chim. Ital.*, 1928, **58**, 231 (*synth*)
Hazlet, S.E. *et al*, *J.A.C.S.*, 1944, **66**, 1781 (*synth*)
Walter, R.I. *et al*, *J. Phys. Chem.*, 1968, **72**, 1217 (*pmr*)
Williams, D.H. *et al*, *J.A.C.S.*, 1969, **91**, 7137 (*ms*)
Milne, G.W.A. *et al*, *J.A.C.S.*, 1971, **93**, 6536 (*nmr*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BMT325, BNF250; (1993 Update), BMR100.
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworth, London and Boston, 1990, 2781.
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, Cambridge, 1992, 169.

Bromo[18]annulene B-0-03743

1-Bromo-1,3,5,7,9,11,13,15,17-cyclooctadecanonaene, 8CI

[29040-89-9]

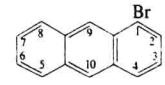


$C_{18}H_{17}Br$ M 313.2
Red-violet cryst. (CH_2Cl_2/petrol). Dec. on attempted Mp determination.

Woo, E.P. *et al*, *Tetrahedron*, 1970, **26**, 3933 (*synth, uv, pmr*)

1-Bromoanthracene B-0-03744

[7397-92-4]



$C_{14}H_9Br$ M 257.1
Cryst. (Et_2O/pentane). Mp 97-100°.

Ohno, I. *et al*, *Bull. Chem. Soc. Jpn.*, 1968, **41**, 2264 (*uv*)
Ahktar, M.N. *et al*, *J.C.S. Perkin 1*, 1979, 1442 (*synth*)
Rickborn, B. *et al*, *J.O.C.*, 1986, **51**, 1189 (*synth, pmr*)

2-Bromoanthracene B-0-03745

[7321-27-9]

$C_{14}H_9Br$ M 257.1
Cryst. (MeOH). Mp 223-224°.

Ohno, I. *et al*, *Bull. Chem. Soc. Jpn.*, 1968, **41**, 2264 (*uv*)
Porzi, G. *et al*, *J. Organomet. Chem.*, 1977, **128**, 95 (*synth*)
Rickborn, B. *et al*, *J.O.C.*, 1986, **51**, 1189 (*synth, pmr*)

9-Bromoanthracene, 9CI B-0-03746

ms-*Bromoanthracene. γ-Bromoanthracene*

[1564-64-3]

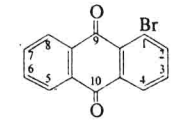
$C_{14}H_9Br$ M 257.1
Yellow needles (EtOH). Mp 100°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 174B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1031D (*ir*)
LeFevre, R. *et al*, *J.C.S.(B)*, 1968, 775 (*props*)
Ohno, I. *et al*, *Bull. Chem. Soc. Jpn.*, 1968, **41**, 2264 (*uv*)
Bartle, K.D., *Tetrahedron*, 1969, **25**, 2701 (*pmr*)
Weinshenker, N.M., *Org. Prep. Proced.*, 1969, **1**, 33 (*synth*)
Brigodiot, M. *et al*, *Spectrochim. Acta A*, 1971, **27**, 1315, 1325 (*ir, Raman*)
Adcock, W. *et al*, *Aust. J. Chem.*, 1974, **27**, 1817 (*cmr*)
House, H.O. *et al*, *J.O.C.*, 1980, **45**, 1807 (*synth, uv, pmr, ms*)
Schuster, I.I., *J.O.C.*, 1981, **46**, 5110 (*cmr*)

1-Bromoanthraquinone B-0-03747

1-Bromo-9,10-anthracenedione, 9CI. α-Bromoanthraquinone

[632-83-7]



$C_{14}H_7BrO_2$ M 287.1
Yellow cryst. (C_6H_6, $PhNO_2$ or xylene). Mp 188°.

v. Pechmann, H., *Ber.*, 1879, **12**, 2124.
Perel'son, M.E. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1964, 804 (*ir*)
Klimasenko, N.L. *et al*, *Kristallografiya*, 1969, **14**, 266 (*cryst struct*)
Tushishvili, L.Sh. *et al*, *Zh. Fiz. Khim.*, 1969, **43**, 981 (*uv*)

2-Bromoanthraquinone B-0-03748

2-Bromo-9,10-anthracenedione, 9CI. β-Bromoanthraquinone

[572-83-8]

$C_{14}H_7BrO_2$ M 287.1
Yellow cryst. (AcOH). Mp 207°.

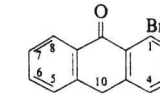
▶ CB5950000.

Heller, G., *Ber.*, 1912, **45**, 665 (*synth*)
Grandmougin, E., *C. R. Hebd. Seances Acad. Sci.*, 1921, **173**, 1176 (*synth*)
Perel'son, M.E. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1964, 804 (*ir*)
Tushishvili, L.Sh. *et al*, *Zh. Fiz. Khim.*, 1969, **43**, 981 (*uv*)

1-Bromoanthrone B-0-03749

1-Bromo-9(10H)-anthracenone, 9CI

[87666-45-3]



$C_{14}H_9BrO$ M 273.1
Yellow cryst. (C_6H_6/hexane). Mp 129-130°.

Yamamoto, G. *et al*, *Bull. Chem. Soc. Jpn.*, 1983, **56**, 2082 (*synth, pmr*)

4-Bromoanthrone B-0-03750

4-Bromo-9(10H)-anthracenone, 9CI

[100790-92-9]

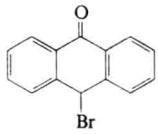
$C_{14}H_9BrO$ M 273.1
Yellow cryst. (MeOH). Mp 137.5-138.5°.

Rickborn, B. *et al*, *J.O.C.*, 1986, **51**, 1189 (*synth, pmr, ms*)

10-Bromoanthrone, 8CI B-0-03751

10-Bromo-9(10H)-anthracenone, 9CI

[1560-32-3]



$C_{14}H_9BrO$ M 273.1

Keto-form (illus.) predominates in $CDCl_3$ soln. Yellow needles (toluene). Mp 148°.

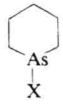
[51678-94-5]

Meyer, K.H., *Annalen*, 1911, **379**, 37 (*synth*)
Koch, W. *et al*, *Helv. Chim. Acta*, 1965, **48**, 554 (*pmr*)
Branz, S.E. *et al*, *Synth. Commun.*, 1986, **16**, 441 (*synth, pmr, tautom*)

1-Bromoarsenane, 9CI B-0-03752

Bromoarsepidine (obsol.). 1-Bromoarsenidene (obsol.). 1-Arsa-1-bromocyclohexane

[129393-84-6]



$C_5H_{10}AsBr$ M 224.9

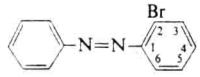
Synth. by heating the complex from 1-methylarsenane and Br_2. Red oil.

Zappi, E.V., *Bull. Soc. Chim. Fr.*, 1931, **49**, 366 (*synth*)
Pasterczyk, J.W. *et al*, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 1990, **48**, 157 (*ms*)

2-Bromoazobenzene B-0-03753

(2-Bromophenyl)phenyldiazene, 9CI

[4103-29-1]



$C_{12}H_9BrN_2$ M 261.1

Golden leaflets. Mp 87°.

Janovsky, M. *et al*, *Ber.*, 1886, **19**, 2156.
Holt, P.F. *et al*, *J.C.S.*, 1965, 5245 (*uv*)
Fahey, D.R., *J. Organomet. Chem.*, 1971, **27**, 283 (*synth, ir*)
Pentimalli, L. *et al*, *Ann. Chim. (Rome)*, 1973, **63**, 749 (*synth*)

3-Bromoazobenzene B-0-03754

(3-Bromophenyl)phenyldiazene, 9CI

[4171-34-0]

$C_{12}H_9BrN_2$ M 261.1

Yellowish-brown leaflets (petrol). Mp 69°.

Janovsky, M. *et al*, *Ber.*, 1887, **20**, 357.
Bowie, J.H. *et al*, *J.C.S.(B)*, 1967, 621 (*ms*)
Ellerhurst, R.H. *et al*, *J.O.C.*, 1968, **33**, 4115 (*uv*)
Yamada, K., *CA*, 1970, **77**, 90028g.
Rehak, V. *et al*, *Coll. Czech. Chem. Comm.*, 1973, **38**, 697.

4-Bromoazobenzene B-0-03755

(4-Bromophenyl)phenyldiazene, 9CI

[4418-84-2]

$C_{12}H_9BrN_2$ M 261.1

(E)-form [6141-96-4]

Orange red cryst. (propanol). Mp 90-91°.

(Z)-form [53547-13-0]

Red oil or dark-red cryst. (petrol). Mp 39°, Mp 47°.

Janovsky, M. *et al*, *Ber.*, 1887, **20**, 357.
Cook, A.H. *et al*, *J.C.S.*, 1939, 1309.
Holt, P.F. *et al*, *J.C.S.*, 1965, 5245 (*uv*)
Bowie, J.H. *et al*, *J.C.S.(B)*, 1967, 621 (*ms*)
Rehak, V. *et al*, *Coll. Czech. Chem. Comm.*, 1973, **38**, 697.
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th edn., Van Nostrand Reinhold, 1979, 432.

2-Bromobenzaldehyde B-0-03756

[6630-33-7]

C_7H_5BrO M 185.0

Cryst. or liq. Mp 22°. Bp 230°, Bp_{12} 118-119°.

(E)-*Oxime:* [52707-51-4].
C_7H_6BrNO M 200.0 Mp 104°.

(E)-*Oxime; hydrochloride:* Mp 115°.

(Z)-*Oxime:* [52707-56-9].
C_7H_6BrNO M 200.0 Mp 126°.

Semicarbazone: Mp 214°.

2,4-Dinitrophenylhydrazone: [34158-85-5]. Mp 203°.

[34158-72-0]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 933C.
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 105B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1284D (*ir*)
Brady, O.L. *et al*, *J.C.S.*, 1925, **127**, 2427 (*synth*)
Angyal, S. *et al*, *J.C.S.*, 1949, 2704.
Yoder, C.H. *et al*, *J.O.C.*, 1976, **41**, 1511 (*cmr*)

3-Bromobenzaldehyde B-0-03757

[3132-99-8]

C_7H_5BrO M 185.0

Bp 233-236°, Bp_2 66-68°.

(E)-*Oxime:* [52739-46-5].
C_7H_6BrNO M 200.0 Mp 74°.

(Z)-*Oxime:* [51873-95-1].
C_7H_6BrNO M 200.0 Cryst. (C_6H_6). Mp 121°.

Semicarbazone: Pale-yellow needles. Mp 205°.

2,4-Dinitrophenylhydrazone: [13034-96-3]. Dec. on heating.

[32605-62-2]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 936B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 108A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1287C (*ir*)
Aldrich Library of IR Spectra, 799D (*ir*)
Aldrich Library of NMR Spectra, **6**, 82A (*pmr*)
Angyal, S.J. *et al*, *J.C.S.*, 1949, 2704 (*synth*)
Pearson, D.E. *et al*, *J.O.C.*, 1958, **23**, 1412 (*synth*)
Jaiswal, R.M.P., *Indian J. Pure Appl. Phys.*, 1969, **7**, 47 (*uv*)
Brown, E.V., *Org. Mass Spectrom.*, 1973, **7**, 1337 (*ms*)
Drakenberg, T. *et al*, *J.C.S. Perkin 2*, 1975, 1682 (*cmr*)

4-Bromobenzaldehyde B-0-03758

[1122-91-4]

C_7H_5BrO M 185.0

Leaflets (H_2O). Mp 59-60°, Mp 67°.

▶ LD_{50} (mus, orl) 1230 mg/kg. CU4810000.

(E)-*Oxime:*
C_7H_6BrNO M 200.0 Cryst. (C_6H_6). Mp 111°.

(Z)-*Oxime:* [25062-46-8].
C_7H_6BrNO M 200.0 Cryst. (C_6H_6). Mp 166-167° (157°).

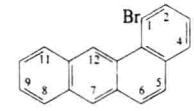
Semicarbazone: [14066-66-1]. Mp 227-229°.

2,4-Dinitrophenylhydrazone: [2087-20-9]. Mp 260-261°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 940C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 110D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1290B (*ir*)
Angyal, S. *et al*, *J.C.S.*, 1949, 2704 (*synth*)
Dalton, D.R. *et al*, *J.O.C.*, 1973, **38**, 4200 (*oximes*)
Brown, E.V. *et al*, *Org. Mass Spectrom.*, 1973, **7**, 1337 (*ms*)
Yanovskaya, L.A. *et al*, *Tetrahedron*, 1973, **29**, 2053 (*uv*)
Bromilow, J. *et al*, *J.C.S. Perkin 2*, 1981, 753 (*cmr*)

1-Bromobenz[*a*]anthracene, 9CI B-0-03759

[78302-32-6]



$C_{18}H_{11}Br$ M 307.1

Cryst. (C_6H_6). Mp 167-168°.

Hallmark, R.K., *J. Labelled Compd. Radiopharm.*, 1981, **18**, 331 (*synth*)

2-Bromobenz[*a*]anthracene, 9CI B-0-03760

[78302-30-4]

$C_{18}H_{11}Br$ M 307.1

Cryst. (C_6H_6). Mp 159.5-161°.

Hallmark, R.K., *J. Labelled Compd. Radiopharm.*, 1981, **18**, 331 (*synth*)
Carmichael, I. *et al*, *J. Phys. Chem. Ref. Data*, 1987, **16**, 239 (*uv*)

3-Bromobenz[*a*]anthracene, 9CI B-0-03761

[78302-31-5]

$C_{18}H_{11}Br$ M 307.1

Cryst. (C_6H_6). Mp 189-191°.

Hallmark, R.K., *J. Labelled Compd. Radiopharm.*, 1981, **18**, 331 (*synth*)

4-Bromobenz[*a*]anthracene, 9CI B-0-03762

[61921-39-9]

$C_{18}H_{11}Br$ M 307.1

Needles (C_6H_6), plates (AcOH). Mp 215-216°.

[61921-52-6]

Badger, G.M. *et al*, *J.C.S.*, 1949, 799 (*synth*)

Bodger, E.O. *et al*, *Acta Cryst. B*, 1977, **33**, 125 (*cryst struct*)
Cho, B.P. *et al*, *J.O.C.*, 1987, **52**, 5668 (*synth, pmr, uv*)

7-Bromobenz[*a*]anthracene, 9CI B-0-03763

$C_{18}H_{11}Br$ M 307.1
Needles or plates (AcOH), pale orange needles. Mp 150-151° (147.5-148.5°).
Picrate: Blood-red, flat needles (AcOH). Mp 155.5-156.5°.

Badger, G.M. *et al*, *J.C.S.*, 1940, 409 (*synth*)
Mikhailov, B.M. *et al*, *Zh. Obshch. Khim.*, 1951, **21**, 2184; *CA*, **46**, 8080a (*synth*)
Yagi, H. *et al*, *J. Labelled Compd. Radiopharm.*, 1976, **12**, 127 (*synth*)
Lee, H.M. *et al*, *J.O.C.*, 1979, **44**, 4948 (*synth*)

Bromobenzene, 9CI B-0-03764

Phenyl bromide
[108-86-1]

PhBr

C_6H_5Br M 157.0
Liq. d_4^{20} 1.495. Mp −30.6°. Bp 156.2°, Bp_5 27.8°.

► Flammable, fl. p. 51/65°, autoignition temp. 565°. Eye and mucous membrane irritant. High vapour conc. may be narcotic. LD_{50} (rat, orl) 2699 mg/kg. CY9000000.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 61C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 971C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 889C (*ir*)
Sadtler Standard Ultraviolet Spectra, 954 (*uv*)
Vogel, A.I., *Practical Organic Chemistry*, 3rd Ed., Longmans, 1959, 535 (*synth*)
McLafferty, F.W., *Anal. Chem.*, 1962, **34**, 2 (*ms*)
Cook, I.B., *Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, PEO500.
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworth, London and Boston, 1990, 2089.
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, Cambridge, 1992, 167.

4-Bromobenzene-diazonium(1+), 9CI B-0-03765

[17333-82-3]

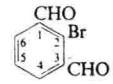
$C_6H_4BrN_2^{\oplus}$ M 184.0
Tetrafluoroborate: [673-40-5].
$C_6H_4BBrF_4N_2$ M 270.8 Cryst. Mp 135° dec.

[2028-85-5]

Grummitt, O. *et al*, *Org. Prep. Proced. Int.*, 1970, **2**, 10 (*synth*)
Doyle, M.P. *et al*, *J.O.C.*, 1979, **49**, 1572 (*synth, pmr*)

2-Bromo-1,3-benzenedicarboxaldehyde, B-0-03766

9CI
2-Bromoisophthalaldehyde, 8CI
[79839-49-9]



$C_8H_5BrO_2$ M 213.0
Pale yellow needles (EtOH). Mp 137.5-138.5°.

Wille, E.E. *et al*, *J.A.C.S.*, 1982, **104**, 405 (*synth, ir, pmr, ms*)

2-Bromo-1,4-benzenedicarboxaldehyde B-0-03767

Bromoterephthalaldehyde
$C_8H_5BrO_2$ M 213.0
Cryst. (H_2O). Mp 75°.
Dioxime:
$C_8H_7BrN_2O_2$ M 243.0 Cryst. (EtOH). Mp 218°.

Hazlet, S.E. *et al*, *J.O.C.*, 1964, **29**, 2034.

4-Bromo-1,2-benzenedicarboxaldehyde, B-0-03768

9CI
4-Bromophthalaldehyde, 8CI
[13209-32-0]
$C_8H_5BrO_2$ M 213.0
Cryst. (Et_2O/petrol). Mp 98-100°.

Mislow, K. *et al*, *J.A.C.S.*, 1962, **84**, 3591 (*synth*)
Kerfanto, M. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 2966 (*synth*)
Pappas, J.J. *et al*, *J.O.C.*, 1968, **33**, 787 (*synth, ir, pmr*)

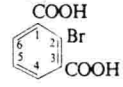
5-Bromo-1,3-benzenedicarboxaldehyde, B-0-03769

9CI
5-Bromoisophthalaldehyde, 8CI
[120173-41-3]
$C_8H_5BrO_2$ M 213.0
Cryst. (Et_2O/EtOAc). Mp 124°.

Netzke, K. *et al*, *Chem. Ber.*, 1989, **122**, 1365 (*synth, ir, pmr, ms*)

2-Bromo-1,3-benzenedicarboxylic acid, B-0-03770

9CI
2-Bromoisophthalic acid, 8CI
[22433-91-6]



$C_8H_5BrO_4$ M 245.0
Mp 218°.
Di-Me ester: [39622-80-5].
$C_{10}H_9BrO_4$ M 273.0 Oil. Bp_{22} 190-191°.
Dinitrile: [22433-90-5]. *2-Bromo-1,3-dicyanobenzene*
$C_8H_3BrN_2$ M 207.0 Mp 190-190.5°.

Coulson, E.A., *J.C.S.*, 1937, 1298 (*synth*)
Fendler, E.J. *et al*, *J.O.C.*, 1970, **35**, 287 (*nitrile*)
Helmchen, G. *et al*, *Helv. Chim. Acta*, 1972, **55**, 2599 (*synth*)
Krizan, T.D. *et al*, *J.O.C.*, 1982, **47**, 2681 (*nitrile*)
Miyano, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 3285 (*synth, ir, pmr*)

2-Bromo-1,4-benzenedicarboxylic acid B-0-03771

Bromoterephthalic acid
[586-35-6]
$C_8H_5BrO_4$ M 245.0
Needles (H_2O). Mp 299°. pK_{a1} 2.21; pK_{a2} 4.10 (25°).
1-Me ester:
$C_9H_7BrO_4$ M 259.0 Cryst. (petrol). Mp 145°. Bp_{37} 235°.
4-Me ester:
$C_9H_7BrO_4$ M 259.0 Yellowish cryst. (petrol). Mp 54°. Bp_{19} 233°.
Di-Me ester:
$C_{10}H_9BrO_4$ M 273.0 Cryst. Mp 54°.
Diamide:
$C_8H_7BrN_2O_2$ M 243.0 Cryst. (EtOH). Mp 270°.
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 1133C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 224C (*ir*)
McIntyre, J.E. *et al*, *J.C.S.*, 1961, 4082 (*synth*)

3-Bromo-1,2-benzenedicarboxylic acid, B-0-03772

9CI
3-Bromophthalic acid, 8CI
[116-69-8]
$C_8H_5BrO_4$ M 245.0
Cryst. (EtOH). Sol. H_2O. Mp 188°. pK_{a1} 2.27; pK_{a2} 4.35 (25°, 0.1*M* KNO_3). Forms anhydride at Mp.
Di-Me ester: [58749-33-0].
$C_{10}H_9BrO_4$ M 273.0 Mp 81-82°. Bp_5 141-145°.
Anhydride:
$C_8H_3BrO_3$ M 227.0 Needles. Mp 132-134°.

v. Braun, J. *et al*, *Ber.*, 1923, **56**, 2332 (*synth*)
Soucy, C. *et al*, *J.O.C.*, 1987, **52**, 129 (*deriv, synth, pmr, cmr, ms*)

4-Bromo-1,2-benzenedicarboxylic acid, B-0-03773

9CI
4-Bromophthalic acid, 8CI
[6968-28-1]
$C_8H_5BrO_4$ M 245.0
Cryst. (xylene). Mp 173-175°. pK_{a1} 2.50; pK_{a2} 4.60 (25°, 0.1*M* KNO_3). Forms anhydride at Mp.
Di-Me ester:
$C_{10}H_9BrO_4$ M 273.0 Cryst. (petrol). Mp 40°. Bp 303-306°.
Dichloride:
$C_8H_3BrCl_2O_2$ M 281.9 Needles (H_2O). Mp 168°.
Anhydride:
$C_8H_3BrO_3$ M 227.0 Needles. Mp 113°. Bp 297-301°.

Pummerer, R. *et al*, *Chem. Ber.*, 1953, **86**, 412 (*synth*)

4-Bromo-1,3-benzenedicarboxylic acid, 9CI B-0-03774

4-Bromoisophthalic acid

[6939-93-1]

$C_8H_5BrO_4$ M 245.0
Needles (EtOH aq.). Mp 303-304° (287°).

Di-Et ester: [56984-35-1].
$C_{12}H_{13}BrO_4$ M 301.1 Oil. Bp_{365} 320-325°.

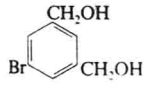
3-Nitrile: 4-Bromo-3-cyanobenzoic acid
$C_8H_4BrNO_2$ M 226.0 Needles. Mp 186°. Sublimes.

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 224D (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., **2**, 221B (*nmr*)
Claus, A., *J. Prakt. Chem.*, 1891, **43**, 355 (*synth*)
Gibson, M.S., *J.C.S.*, 1956, 776 (*synth*)

5-Bromo-1,3-benzenedimethanol B-0-03775

1-Bromo-3,5-bis(hydroxymethyl)benzene

[51760-22-6]



$C_8H_9BrO_2$ M 217.0
Cryst. (C_6H_6). Mp 90-91°.

Sherrod, S.A. *et al*, *J.A.C.S.*, 1974, **96**, 1565 (*synth, pmr, ms*)

2-Bromo-1,3-benzenediol, 9CI B-0-03776

2-Bromoresorcinol, 8CI

[6751-75-3]

$C_6H_5BrO_2$ M 189.0
Cryst. ($CHCl_3$/petrol). Mp 102-103°.

Davis, T.L. *et al*, *J.A.C.S.*, 1934, **56**, 129 (*synth*)
Dell, H.D. *et al*, *Annalen*, 1967, **709**, 70 (*spectra*)

2-Bromo-1,4-benzenediol, 9CI B-0-03777

Bromohydroquinone, 8CI. Bromoquinol. Adurol

[583-69-7]

$C_6H_5BrO_2$ M 189.0
Isol. from various acorn worms.
Photographic developer. Cryst. (toluene). Sol. H_2O. Mp 110-111°. pK_{a1} 8.67; pK_{a2} 10.68 (22°, KCl). Sublimes.

► CZ8920000.

Di-Ac: [52376-16-6].
$C_{10}H_9BrO_4$ M 273.0 Mp 71-73°.

Di-Me ether: [25245-34-5]. *2-Bromo-1,4-dimethoxybenzene*
$C_8H_9BrO_2$ M 217.0 Oil. Bp 262-263°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 199B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1048D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 980B (*ir*)
Bilmann, E. *et al*, *J.C.S.*, 1925, **127**, 205 (*synth*)
Yanovskaya, L.A. *et al*, *Zh. Obshch. Khim.*, 1952, **22**, 1594; *CA*, **47**, 8032 (*synth*)
Higa, T. *et al*, *Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **65**, 525 (*isol*)
Pinault, M. *et al*, *Synthesis*, 1990, 935 (*synth*)

3-Bromo-1,2-benzenediol, 9CI B-0-03778

3-Bromopyrocatechol, 8CI. 3-Bromocatechol

[14381-51-2]

$C_6H_5BrO_2$ M 189.0
Mp 40.5-41.5°. Bp_9 118-120°. pK_a 9.40 (40% dioxan aq.).

Di-Ac:
$C_{10}H_9BrO_4$ M 273.0 Mp 83-84°.

1-Me ether: [28165-49-3]. *2-Bromo-6-methoxyphenol. 6-Bromoguaiacol*
$C_7H_7BrO_2$ M 203.0 Cryst. (MeOH). Mp 63°.

Di-Me ether: [5424-43-1]. *1-Bromo-2,3-dimethoxybenzene. 3-Bromoveratrole*
$C_8H_9BrO_2$ M 217.0 Bp_5 114°.

Robertson, P.W., *J.C.S.*, 1908, **93**, 788.
Simonsen, J.L. *et al*, *J.C.S.*, 1918, **113**, 782.
Mann, H.S., *J.A.C.S.*, 1947, **69**, 224.
Case, S. *et al*, *J.A.C.S.*, 1951, **73**, 5706.
Stevens, R.V. *et al*, *J.O.C.*, 1982, **47**, 2393 (*synth, pmr*)

4-Bromo-1,2-benzenediol, 9CI B-0-03779

4-Bromopyrocatechol, 8CI. 4-Bromocatechol

[17345-77-6]

$C_6H_5BrO_2$ M 189.0
Mp 87°. pK_{a1} 8.7; pK_{a2} 12.4 (25°, 0.1*M* KCl).

Di-Ac: [66373-95-3].
$C_{10}H_9BrO_4$ M 273.0 Mp 109°.

1-Me ether: [37942-01-1]. *5-Bromo-2-methoxyphenol. 5-Bromoguaiacol*
$C_7H_7BrO_2$ M 203.0 Prisms (petrol). Mp 65°. Bp_{20} 150°.

2-Me ether: [7368-78-7]. *4-Bromo-2-methoxyphenol. 4-Bromoguaiacol*
Needles. Mp 46°. Bp_{60} 181-182°.

Di-Me ether: [2859-78-1]. *4-Bromo-1,2-dimethoxybenzene. 4-Bromoveratrole*
$C_8H_9BrO_2$ M 217.0 Bp 255-256°, Bp_{30} 157-158°.

1,2-Methylene ether: see *5-Bromo-1,3-benzodioxole, B-0-03812*

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 198C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1048B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 979C (*ir*)
Hindmarsh, E.M. *et al*, *J.C.S.*, 1917, 940.
Rosenmund, K.W. *et al*, *Ber.*, 1923, **56**, 1262 (***synth***, *pmr*)
Sloof, G., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1935, **54**, 995.

4-Bromo-1,3-benzenediol, 9CI B-0-03780

4-Bromoresorcinol, 8CI

[6626-15-9]

$C_6H_5BrO_2$ M 189.0
Used as a 5% aq. soln. for photometric detn. of Zn (λ_{max} 630 nm). Cryst. (EtOH). Sol. H_2O. Mp 100-102°.

Di-Ac: [66417-41-2].
$C_{10}H_9BrO_4$ M 273.0 Mp 49-50°.

1-Me ether: [63604-94-4]. *2-Bromo-5-methoxyphenol*
$C_7H_7BrO_2$ M 203.0 Oil. Bp_{25} 152°.

3-Me ether: 4-Bromo-3-methoxyphenol
$C_7H_7BrO_2$ M 203.0 Needles (C_6H_6). Mp 84°.

Di-Me ether: [17715-69-4]. *1-Bromo-2,4-dimethoxybenzene*
$C_8H_9BrO_2$ M 217.0 Oil. Bp_{18} 135°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 199A, 302A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1048C, 1105D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 980A (*ir*)
Org. Synth., Coll. Vol., 2, 1943, 100 (*synth*)
Stewart, J.A. *et al*, *Anal. Chem.*, 1958, **30**, 404 (*detn. Zn*)

5-Bromo-1,3-benzenediol, 9CI B-0-03781

5-Bromoresorcinol, 8CI

$C_6H_5BrO_2$ M 189.0
Cryst. (C_6H_6). Mp 87°.

Dean, F.M. *et al*, *J.C.S.*, 1954, 4638 (*synth*)

2-Bromobenzenesulfonic acid, 9CI B-0-03782

[576-92-1]

$C_6H_5BrO_3S$ M 237.0
Deliquescent needles.

Chloride: [2905-25-1].
$C_6H_4BrClO_2S$ M 255.5 Cryst. (Et_2O). Mp 51°.

Amide:
$C_6H_6BrNO_2S$ M 236.0 Needles (H_2O). Mp 186°.

Bahlmann, A., *Annalen*, 1876, **181**, 203.
Truce, W.E. *et al*, *J.A.C.S.*, 1951, **73**, 3013.
Jackson, G.R. *et al*, *J.A.C.S.*, 1955, **77**, 5625.

3-Bromobenzenesulfonic acid, 9CI B-0-03783

[22033-09-6]

$C_6H_5BrO_3S$ M 237.0
Deliquescent cryst.

Amide:
$C_6H_6BrNO_2S$ M 236.0 Needles (H_2O). Mp 154°.

Twist, R.F. *et al*, *J.C.S.*, 1925, **127**, 1248 (*synth*)
Jackson, G.R. *et al*, *J.A.C.S.*, 1955, **77**, 5625.

4-Bromobenzenesulfonic acid, 9CI B-0-03784

[138-36-3]

$C_6H_5BrO_3S$ M 237.0
Deliquescent needles ($CHCl_3$). Mp 102-103°. pK_a −3.1 (H_2O).

Me ester: [6213-85-0].
$C_7H_7BrO_3S$ M 251.1 Platelets (MeOH). Mp 60°. Bp_{15} 176°.

Et ester: [20846-02-0].
$C_8H_9BrO_3S$ M 265.1 Platelets (EtOH). Mp 39.5°. Bp_{15} 181-182°, $Bp_{0.15}$ 111-113°.

Chloride: [98-58-8].
$C_6H_4BrClO_2S$ M 255.5 Derivatisation reagent used in gc. anal. of carbamate pesticides. Cryst. (petrol). Mp 77°.

Bromide: [1950-71-6].
$C_6H_4Br_2O_2S$ M 299.9 Cryst. (Et_2O). Mp 77°.

Anhydride: [14248-47-6].

$C_{12}H_8Br_2O_5S_2$ M 456.1 Cryst. (Et_2O). Mp 164-167° dec.

Amide: [701-34-8].
$C_6H_6BrNO_2S$ M 236.0 Cryst. (H_2O). Mp 166.5°.
▶ LD_{50} (mus, orl) 1700 mg/kg. DB0550000.

Anilide: [7454-54-8].
$C_{12}H_{10}BrNO_2S$ M 312.1 Mp 119°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 1621B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 521A (*ir*)
Rây, J.N. *et al*, *J.C.S.*, 1920, **117**, 1405.
Jackson, G.R. *et al*, *J.A.C.S.*, 1955, **77**, 5625.
Moyer, H.A., *J. Agric. Food Chem.*, 1975, **23**, 415 (*use*)
Hamada, T. *et al*, *Synthesis*, 1986, 852 (*deriv, synth, pmr, ms*)

2-Bromobenzenethiol, 9CI B-0-03785

2-Bromophenyl mercaptan. o-*Bromothiophenol*

[6320-02-1]

C_6H_5BrS M 189.0
Bp_6 90-93°.

Ac:
C_8H_7BrOS M 231.1 Bp_{15} 145°.

S-*Me:* [19614-16-5]. *1-Bromo-2-(methylthio) benzene*
C_7H_7BrS M 203.1 Oil. Fp −24.5°. Bp_{768} 256°, Bp_{13-14} 172-179°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 419A, 434C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1175A, 1182C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1091B, 1101B (*ir*)
Saggiomo, A.J. *et al*, *J.O.C.*, 1958, **23**, 1906 (*synth*)

3-Bromobenzenethiol B-0-03786

3-Bromophenyl mercaptan. m-*Bromothiophenol*

[6320-01-0]

C_6H_5BrS M 189.0
Bp_{20-22} 119-121°. pK_a 6.77 (25°, 48% EtOH).

S-*Me:* [33733-73-2]. *1-Bromo-3-(methylthio) benzene*
C_7H_7BrS M 203.1 Bp_1 83-85°.

S-*Et:* [18184-69-5]. *1-Bromo-3-(ethylthio) benzene*
C_8H_9BrS M 217.1 Bp_{11} 122-123°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 421A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1177A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1093D (*ir*)
Wilson, H.F. *et al*, *J.A.C.S.*, 1950, **72**, 5200 (*synth*)
Bordwell, F.G. *et al*, *J.A.C.S.*, 1953, **75**, 6019 (*synth*)
Nodiff, E.A. *et al*, *J.O.C.*, 1960, **25**, 60 (*synth, deriv*)
Miller, S.I. *et al*, *J.O.C.*, 1962, **27**, 645 (*uv*)

4-Bromobenzenethiol, 9CI B-0-03787

4-Bromophenyl mercaptan. p-*Bromothiophenol*

[106-53-6]

C_6H_5BrS M 189.0
Mp 75°. Bp 239°. pK_a 6.99 (25°, 48% EtOH).

Ac: [28122-76-1].
C_8H_7BrOS M 231.1 Cryst. (MeOH). Mp 51-52°.
▶ LD_{50} (mus, orl) 3000 mg/kg. AJ5900000.

S-*Me:* [104-95-0]. *1-Bromo-4-(methylthio) benzene*
C_7H_7BrS M 203.1 Cryst. (MeOH). Mp 38-40°. Bp 255°.

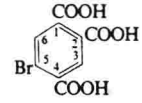
S-*Et:* [30506-30-0]. *1-Bromo-4-(ethylthio) benzene*
C_8H_9BrS M 217.1 $Bp_{0.01}$ 67-70°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 423C, 437B.
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1178B, 1182D.
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1095B, 1101D (*ir*)
Kharasch, N. *et al*, *J.O.C.*, 1954, **19**, 1704 (*synth*)
Miller, S.I. *et al*, *J.O.C.*, 1962, **27**, 645 (*uv*)
Walker, D. *et al*, *J.O.C.*, 1962, **27**, 4455 (*synth*)
Senoff, C.V. *et al*, *Inorg. Chem.*, 1975, **14**, 278 (*cmr*)

5-Bromo-1,2,4-benzenetricarboxylic acid B-0-03788

5-Bromotrimellitic acid

[13124-84-0]



$C_9H_5BrO_6$ M 289.0
Cryst. (EtOAc/hexane). Mp 203-208° (solidifies and remelts at 219-220°).

Tri-Me ester: [13124-85-1].
$C_{12}H_{11}BrO_6$ M 331.1 Needles (hexane). Mp 49-51°.

Moriconi, E.J. *et al*, *J.O.C.*, 1967, **32**, 2829 (*synth, ir, nmr*)

6-Bromo-1,2,4-benzenetricarboxylic acid B-0-03789

6-Bromotrimellitic acid

$C_9H_5BrO_6$ M 289.0
Cryst. Mp 237°.

2,4-Di-Me ester:
$C_{11}H_9BrO_6$ M 317.0 Needles (H_2O). Mp 130-131°.

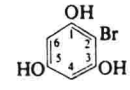
Tri-Me ester:
$C_{12}H_{11}BrO_6$ M 331.1 Needles (MeOH). Mp 110°.

Zincke, Th. *et al*, *Annalen*, 1896, **293**, 149.

2-Bromo-1,3,5-benzenetriol, 9CI B-0-03790

2-Bromophloroglucinol

[84743-77-1]



$C_6H_5BrO_3$ M 205.0
Isol. from *Rhabdonia verticillata.*

Tri-Ac: [96820-10-9].
$C_{12}H_{11}BrO_6$ M 331.1 Isol. from *Eisenia arborea.* No phys. props. reported.

Tri-Me ether: [1131-40-4]. *2-Bromo-1,3,5-trimethoxybenzene, 9CI*
$C_9H_{11}BrO_3$ M 247.0 Cryst. (Et_2O). Mp 99°.

Blackman, A.J. *et al*, *Phytochemistry*, 1982, **21**, 2141 (*isol*)
Fischer, A. *et al*, *Can. J. Chem.*, 1983, **61**, 1045 (*deriv*)
Glombitza, K.W. *et al*, *Phytochemistry*, 1985, **24**, 543 (*deriv*)

3-Bromo-1,2,4-benzenetriol B-0-03791

[99910-88-0]

$C_6H_5BrO_3$ M 205.0

Tri-Me ether: [25245-41-4]. *2-Bromo-1,3,4-trimethoxybenzene*
$C_9H_{11}BrO_3$ M 247.0 Cryst. (pentane). Mp 77-78°.

Bacon, R.G.R. *et al*, *J.C.S.(C)*, 1969, 1978 (*synth, deriv, pmr*)
Arias, S. *et al*, *Electrochim. Acta*, 1985, **30**, 1441.

4-Bromo-1,2,3-benzenetriol, 9CI B-0-03792

4-Bromopyrogallol, 8CI

[17345-72-1]

$C_6H_5BrO_3$ M 205.0
Mp 119-120°.

1,3-Di-Me ether: [18111-34-7]. *3-Bromo-2,6-dimethoxyphenol, 8CI*
$C_8H_9BrO_3$ M 233.0 $Bp_{0.4}$ 88°.

Tri-Me ether: [10385-36-1]. *1-Bromo-2,3,4-trimethoxybenzene, 9CI*
$C_9H_{11}BrO_3$ M 247.0 Bp_{13} 148°, $Bp_{0.5}$ 97°.

Friedman, D. *et al*, *J.O.C.*, 1958, **23**, 16 (*synth*)
Goldman, J. *et al*, *Tetrahedron*, 1973, **29**, 3833 (*deriv*)
Manwell, M.G. *et al*, *Aust. J. Chem.*, 1992, **45**, 1967 (*deriv*)

5-Bromo-1,2,3-benzenetriol, 9CI B-0-03793

5-Bromopyrogallol, 8CI

[16492-75-4]

$C_6H_5BrO_3$ M 205.0
Off-white needles ($CHCl_3$). Mp 148°.

1,3-Di-Me ether: [70654-71-6]. *4-Bromo-2,6-dimethoxyphenol, 9CI*
$C_8H_9BrO_3$ M 233.0 Mp 99.5-100°.

Tri-Me ether: [2675-79-8]. *5-Bromo-1,2,3-trimethoxybenzene, 9CI*
$C_9H_{11}BrO_3$ M 247.0 Cryst. (hexane). Mp 82-83° (78°).

Critchlow, A. *et al*, *Tetrahedron*, 1967, **23**, 2829 (*synth*)
Jung, M.E. *et al*, *J.O.C.*, 1985, **50**, 1087 (*derivs*)
Banwell, M.G. *et al*, *Aust. J. Chem.*, 1992, **45**, 1967 (*tri-Me ether*)

5-Bromo-1,2,4-benzenetriol B-0-03794

$C_6H_5BrO_3$ M 205.0

Tri-Ac: [23046-47-1].
$C_{12}H_{11}BrO_6$ M 331.1 Cryst. (EtOH). Mp 116.5-117.5°.

Tri-Me ether: [20129-11-7]. *1-Bromo-2,4,5-trimethoxybenzene*
$C_9H_{11}BrO_3$ M 247.0 Cubes (petrol). Mp 54-55°.

Fabinyi, R. *et al*, *Chem. Ber.*, 1910, **43**, 2676.

Blatchly, J.M. *et al*, *J.C.S.(C)*, 1969, 1350 (*synth, pmr*)
Bacon, R.G.R. *et al*, *J.C.S.(C)*, 1969, 1978 (*synth*)

6-Bromo-1,2,4-benzenetriol B-0-03795

$C_6H_5BrO_3$ M 205.0
Amorph. powder. Mp 137-139°.

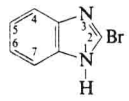
Tri-Ac: [38475-38-6].
$C_{12}H_{11}BrO_6$ M 331.1 Mp 73-74°.

Tri-Me ether: [23030-39-9]. *1-Bromo-2,3,5-trimethoxybenzene*
$C_9H_{11}BrO_3$ M 247.0 Oil. Bp_1 117-119°.

Hughes, G.K. *et al*, *Aust. J. Sci. Res., Ser. A*, 1950, **3**, 497 (*synth, deriv*)
Blatchly, J.M., *J.C.S.(C)*, 1972, 2286 (*deriv*)
Sanchez, I.H. *et al*, *Tetrahedron*, 1985, **41**, 2355 (*synth, deriv, uv, ir, pmr, cmr*)
Sinhababu, A.K. *et al*, *J. Het. Chem.*, 1988, **25**, 1155 (*synth, deriv, pmr*)

2-Bromo-1*H*-benzimidazole, 9CI B-0-03796

[54624-57-6]



$C_7H_5BrN_2$ M 197.0
Cryst. (Me_2CO). Mp 190-192°.

1-Me: [49572-60-3].
$C_8H_7BrN_2$ M 211.0 Cryst. (Et_2O). Mp 103-105°.

Ellingboe, J.W. *et al*, *J. Med. Chem.*, 1992, **35**, 705 (*synth, pmr*)

5-Bromo-1*H*-benzimidazole, 9CI B-0-03797

[4887-88-1]

$C_7H_5BrN_2$ M 197.0
Cryst. Mp 130-131°.

Rabiger, D.J. *et al*, *J.C.S.*, 1964, 915 (*synth*)

1-Bromobenzo[*c*]cinnoline B-0-03798

[13111-94-9]

$C_{12}H_7BrN_2$ M 259.1
Pale-yellow needles (MeOH). Mp 121-122° (199°).

5-Oxide: Small pale yellow needles. Mp 156-158°.

6-Oxide: Large pale yellow needles. Mp 202-204°. An *N*-oxide (posn. of oxidn. indetermined) Mp 225-227° was reported by Corbett.

Corbett, J.F. *et al*, *J.C.S.*, 1961, 5029; 1962, 1812 (*synth, oxide*)
Holt, P.F. *et al*, *J.C.S.(C)*, 1966, 1306 (*oxide*)
Barton, J.W. *et al*, *J.C.S. Perkin 1*, 1979, 1503 (*synth, pmr*)

2-Bromobenzo[*c*]cinnoline B-0-03799

[72005-78-8]

$C_{12}H_7BrN_2$ M 259.1
Dull yellow needles (C_6H_6 or EtOH). Mp 221-222°.

5-Oxide:
$C_{12}H_7BrN_2O$ M 275.1 Mp 230-232°.

6-Oxide: [94522-80-2].
$C_{12}H_7BrN_2O$ M 275.1 Cryst. (CH_2Cl_2/petrol). Mp 251-252°.

Corbett, J.F. *et al*, *J.C.S.*, 1961, 5029; 1962, 1812.
Barton, J.W. *et al*, *J.C.S. Perkin 1*, 1979, 1503 (*pmr*)
Kilic, E. *et al*, *Org. Prep. Proced. Int.*, 1990, **22**, 485 (*synth, bibl*)

3-Bromobenzo[*c*]cinnoline B-0-03800

3-Bromophenazone. 3-Bromo-5,6-phenanthroline

[72005-79-9]

$C_{12}H_7BrN_2$ M 259.1
Shows herbicidal props. Pale-yellow needles (MeOH). Mp 194-195° (191°).

Corbett, J.F. *et al*, *J.C.S.*, 1961, 5029; 1962, 1812 (*synth, uv*)
Barton, J.W. *et al*, *J.C.S. Perkin 1*, 1979, 1503 (*synth, pmr*)
Kilic, E. *et al*, *Org. Prep. Proced. Int.*, 1990, **22**, 485 (*synth*)

4-Bromobenzo[*c*]cinnoline B-0-03801

[13070-08-1]

$C_{12}H_7BrN_2$ M 259.1
Cryst. (2-propanol) or yellow needles (EtOH). Mp 199-200°.

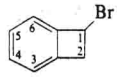
6-Oxide: [13070-13-8].
$C_{12}H_7BrN_2O$ M 275.1 Cryst. (CH_2Cl_2/EtOAc) or pale yellow needles (EtOH). Mp 244-245° (234-235°).

Barton, J.W. *et al*, *J.C.S.*, 1964, 1265 (*synth, oxide, uv*)
Holt, P.F. *et al*, *J.C.S.(C)*, 1966, 1306 (*synth, oxide, uv*)
Barton, J.W. *et al*, *J.C.S. Perkin 1*, 1979, 1503 (*pmr*)
Kilic, E. *et al*, *Org. Prep. Proced. Int.*, 1990, **22**, 485 (*synth, bibl*)

1-Bromobenzocyclobutene B-0-03802

7-Bromobicyclo[4.2.0]octa-1,3,5-triene, 9CI

[21120-91-2]



C_8H_7Br M 183.0
CA numbering differs.

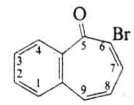
(±)-form
Liq. $Bp_{1.0}$ 55-59°.

Cava, M.P. *et al*, *J.A.C.S.*, 1958, **80**, 2255 (*synth*)
Horner, L. *et al*, *Chem. Ber.*, 1958, **91**, 430.
Fraenkel, G. *et al*, *Tetrahedron*, 1964, **20**, 1179 (*pmr, struct*)
de Camp, M.R. *et al*, *J.O.C.*, 1981, **46**, 3918 (*synth*)
Barton, J.W. *et al*, *J.C.S. Perkin 1*, 1987, 1561 (*synth*)

6-Bromo-5*H*-benzocyclohepten-5-one B-0-03803

7-Bromo-2,3-benzotropone

[22360-00-5]



$C_{11}H_7BrO$ M 235.0
Pale yellow prisms (petrol). Mp 79-80°. Other authors wrongly descr. the 8-isomer as this compd.

Collington, E.W. *et al*, *J.C.S.(C)*, 1969, 2656 (*synth, uv, ir, pmr*)
Moncur, M.V. *et al*, *Chem. Comm.*, 1972, 667 (*bibl*)

8-Bromo-5*H*-benzocyclohepten-5-one B-0-03804

5-Bromo-2,3-benzotropone

[32317-17-2]

$C_{11}H_7BrO$ M 235.0
Pale yellow needles (MeOH). Mp 102-103.5°. This compd. was wrongly descr. as the 6-isomer by other authors.

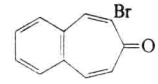
2,4-Dinitrophenylhydrazone: Red needles (EtOAc). Mp 232-233°.

Ebine, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1971, **44**, 3480 (*synth, pmr*)
Moncur, M.V. *et al*, *Chem. Comm.*, 1972, 667 (*synth, bibl*)

6-Bromo-7*H*-benzocyclohepten-7-one, 9CI B-0-03805

2-Bromo-4,5-benzotropone

[5063-84-3]



$C_{11}H_7BrO$ M 235.0
Needles (petrol or by subl.). Mp 142-143° (135°).

Oxime:
$C_{11}H_8BrNO$ M 250.0 Light yellow needles (EtOH aq.). Mp 201-202° (196-198°).

Saraf, S.D., *Can. J. Chem.*, 1969, **47**, 1169 (*synth, uv, ir*)
Saxena, M.K. *et al*, *J. Indian Chem. Soc.*, 1969, **46**, 855 (*synth, ir, uv*)
Yildiz, Y.K. *et al*, *J.O.C.*, 1993, **58**, 5355 (*synth, pmr, ir*)

2-Bromobenzocyclopropene B-0-03806

2-Bromobicyclo[4.1.0]hepta-1,3,5-triene

C_7H_5Br M 169.0
Oil.

Halton, B. *et al*, *Aust. J. Chem.*, 1987, **40**, 475 (*synth, ir, pmr, cmr*)

3-Bromobenzocyclopropene B-0-03807

3-Bromobicyclo[4.1.0]hepta-1,3,5-triene, 9CI

[63370-07-0]

C_7H_5Br M 169.0