Dictionary of Organic Compounds

SIXTH EDITION

VOLUME THREE

Dic–Exo

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D–0-03159–E-0-01265

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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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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.

Dicarbon dioxide D-0-03159

Carbon oxide (C_2O_2). Ethenedione, 9CI

[4363-38-6]

OC=CO

C_2O_2 M 56.0

Not known. Calcns. suggest extreme instability.

Bis(dimethyl acetal): see *Tetramethoxyethene, T-0-02061*

Bis(diethyl acetal): see *Tetraethoxyethene, T-0-00743*

Hoffman, R.W. *et al, Tetrahedron*, 1965, **21**, 891.

Herberhold, M. *et al, Z. Naturforsch., B*, 1976, **31**, 35.

Dicarbonic acid, 9CI D-0-03160

Oxydiformic acid, 8CI. Pyrocarbonic acid. Oxybisformic acid

[503-81-1]

HOOC—O—COOH

$C_2H_2O_5$ M 106.0

Di-Me ester: [4525-33-1]. *Dimethyl dicarbonate. Dimethyl pyrocarbonate. Velcorin*

$C_4H_6O_5$ M 134.0 Yeast inhibitor and preservative for alcoholic beverages. Bp_5 44-47°. n_D^{20} 1.3948.

Di-Et ester: [1609-47-8]. *Diethyl dicarbonate. Diethyl pyrocarbonate. Baycovin*

$C_6H_{10}O_5$ M 162.1 Preservative for beverages, food additive. Reagent for the gc sepn. of amines as urethanes. d_4^{20} 1.12. Bp_3 58.5-62°. n_D^{25} 1.3975.

▶ Poss. protocarcinogen (forms carcinogenic ethyl carbamate with dietary $NH_4^{\oplus}$). Eye, skin and mucous membrane irritant. LD_{50} (rat, orl) 850 mg/kg. LQ9350000.

Di-tert-butyl ester: [4525-32-0]. *Di-tert-butyl dicarbonate. Di-tert-butyl pyrocarbonate*

$C_{10}H_{18}O_5$ M 218.2 Coupling reagent in organic synth. Reagent for introduction of *tert*-butyloxycarbonyl protecting group. Used in protection of pyrroles and indoles and for high yield synth. of Boc-amino acids. Liq. Mp 21-22°. Bp_3 73-75°. n_D^{25} 1.4071, 1.4085.

Dibenzyl ester: [31139-36-3]. *Dibenzyl dicarbonate. Dibenzyl pyrocarbonate*

$C_{16}H_{14}O_5$ M 286.2 Reagent for prepn. of *N*-benzyloxycarbonyl protected amino acids. Cryst. (hexane). Mp 28°.

Di(2-propenyl) ester: [115491-93-5]. *Diallyl dicarbonate. Diallyl pyrocarbonate*

$C_8H_{10}O_5$ M 186.1 Reagent for protection of amino-sugars, aminoacids and nucleosides. $Bp_{0.05}$ 65°. Stable at r.t.

[24424-99-5]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **1**, 929B, 929C (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., **1**, 611B (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 634B, 634C (*ir*)

Rosnati, L., *Chem. Ber.*, 1963, **96**, 3098 (*synth, di-Et ester*)

Fr. Pat., 1 542 382, (1968); *CA*, **71**, 123555h (*manuf, di-Me ester*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 128; 1979, **7**, 91; 1980, **8**, 145; 1982, **10**, 122; 1986, **12**, 159; 1990, **15**, 113 (*use*)

Gejvall, T., *J. Chromatogr.*, 1974, **90**, 157 (*use, Et ester*)

Brysova, V.P. *et al, J.O.C., USSR*, 1974, **10**, 2551 (*synth, di-Me ester*)

Turczan, J.W. *et al, J. Agric. Food Chem.*, 1977, **25**, 594 (*pmr, di-Et ester*)

Org. Synth., 1977, **57**, 45 (*di tert-butyl ester*)

Pope, B.M. *et al, J.O.C.*, 1978, **43**, 2410 (*di-tert-butyl ester*)

Grehn, L. *et al, Angew. Chem., Int. Ed.*, 1984, **23**, 296; 1985, **24**, 510 (*use*)

Pauli, G.H., *J. Chem. Educ.*, 1984, **61**, 332 (*rev, di-Et ester*)

Sennyey, G. *et al, Tet. Lett.*, 1986, **27**, 5375; 1987, **28**, 5809 (*diallyl, dibenzyl esters*)

Lewis, R.J., *Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DRJ850.

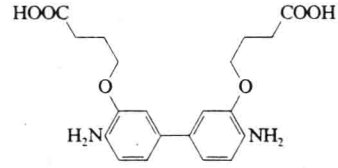
McNulty, J. *et al, Synth. Commun.*, 1992, **22**, 979 (*use, deriv*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DIZ100.

Dicarboxidine D-0-03161

4,4′-[(4,4′-Diamino[1,1′-biphenyl]-3,3′-diyl) bis(oxy)]bisbutanoic acid, 9CI. γ,γ′-(4,4′-Diamino-3,3′-biphenylenedioxy)dibutyric acid

[34915-18-9]



$C_{20}H_{24}N_2O_6$ M 388.4

Used as a 1.25% aq. soln. for photometric detn. of $CN^{\ominus}$, Cl_2. Peroxidase substrate; used in TLC detn. of amino acids, peptides and barbiturates. Microcryst. powder. Mod. sol. H_2O, dil. alkalis. Dec. without definite Mp at ~ 160°.

Hydrochloride (1:2): [56455-90-4]. Cryst. (2*M* HCl). Mp 165° dec.

▶ EK7770000.

Jönsson, N.A. *et al, Acta Chem. Scand., Ser. B*, 1978, **32**, 317 (*synth*)

Gröningsson, K., *Analyst (London)*, 1979, **104**, 367.

Svahn, C.M. *et al, J. Chromatogr.*, 1979, **170**, 292, 294 (*tlc*)

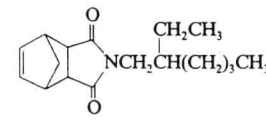
Paul, K.G. *et al, Anal. Biochem.*, 1982, **124**, 102 (*peroxidase*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DEK000.

Dicarboximide D-0-03162

2-(2-Ethylhexyl)-3a,4,7,7a-tetrahydro-4,7-methano-1H-isoindole-1,3(2H)-dione, 9CI. N-(2-Ethylhexyl)-8,9,10-trinorborn-5-ene-2,3-dicarboximide. N-Octylbicycloheptenedicarboximide. Van Dyke 264

[113-48-4]



$C_{17}H_{25}NO_2$ M 275.3

▶ RB8575000.

(±)-form

Insecticidal synergist for pyrethroids. Liq. d^{20} 1.04. Mp < −20°.

▶ LD_{50} (rat, orl) 2800 mg/kg; LD_{50} (rat, skn) 470 mg/kg.

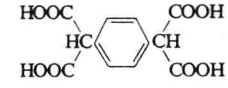
U.S. Pat., 2 476 512, (1947); *CA*, **44**, 5394i.

Pesticide Manual, 9th edn., 1991, No. 5840.

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, OES000.

α,α′-Dicarboxy-1,4-benzenediacetic acid D-0-03163

p-Phenylenedimalonic acid. p-Benzenedimalonic acid



$C_{12}H_{10}O_8$ M 282.2

Tetra-Me ester: p-*Phenylenebis(dimethyl malonate)*

$C_{16}H_{18}O_8$ M 338.3 Cryst. (C_6H_6/pentane). Mp 151.5-152°.

Tetranitrile: [18643-56-6]. *α,α'-Dicyano-1,4-benzenediacetonitrile, 9CI.* p-*Phenylene dimalonitrile*

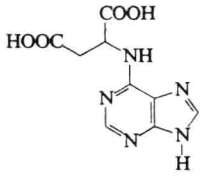
$C_{12}H_6N_4$ M 206.2 Needles (H_2O) or platelets. Mp 246-248°.

Acker, D.S. *et al, J.A.C.S.*, 1962, **84**, 3370 (*deriv, synth, ir, use*)
Uno, M. *et al, Tet. Lett.*, 1985, **26**, 1553 (*synth*)

6-(1,2-Dicarboxyethylamino) purine D-0-03164

N-*1H-Purin-6-ylaspartic acid, 9CI*

[26511-42-2]



$C_9H_9N_5O_4$ M 251.2
Isol. from *Fusarium* sp.

[26287-66-1]

Ballio, A. *et al, Gazz. Chim. Ital.*, 1964, **94**, 156 (*isol*)
McCloskey, J.A. *et al, Biomed. Mass Spectrom.*, 1975, **2**, 90 (*ms*)

S-(1,2-Dicarboxyethyl) glutathione D-0-03165

[[2-[(4-*Amino-4-carboxy-1-oxobutyl)amino*]-3-[(*carboxymethyl)amino*]-3-*oxopropyl*]*thio*] *butanedioic acid, 9CI*

[1115-52-2]

$C_{14}H_{21}N_3O_{10}S$ M 423.4
Peptide present in calf lens tissue.

Waley, S.G. *et al, Biochem. J.*, 1963, **86**, 226 (*isol, struct, synth*)
Ger. Pat., 2 245 903, (1973); *CA*, **79**, 5603q (*synth*)

(1,2-Dicarboxyethyl) triphenylphosphonium(1+) D-0-03166

$Ph_3P^{\oplus}CH(COOH)CH_2COOH$

$C_{22}H_{20}O_4P^{\oplus}$ M 379.3 (ion)
2M NaOH aq. causes dec. of salts to Ph_3PO and succinic acid.

Chloride: [64598-21-6].
$C_{22}H_{20}ClO_4P$ M 414.8 Cryst. (MeOH/EtOAc). Mp 125-130° dec. Possibly decarboxylates to some extent on recryst.

Bromide: [64598-17-0].
$C_{22}H_{20}BrO_4P$ M 459.2 Cryst. + $1H_2O$. Mp 140° dec.

Di-Et ester, iodide:
$C_{26}H_{28}IO_4P$ M 562.3 Cryst. + $1H_2O$. Mp 104°.

Ylide: see (*Triphenylphosphoranylidene*) *butanedioic acid, T-0-06420*

Hoffmann, H., *Chem. Ber.*, 1961, **94**, 1331 (*bromide, ester, props*)
Hudson, R.F. *et al, Helv. Chim. Acta*, 1963, **46**, 2178 (*chloride, props*)

Dichlofluanid, BSI D-0-03167

*1,1-Dichloro-*N-[(*dimethylamino)sulfonyl*]-*1-fluoro-*N-*phenylmethanesulfenamide, 9CI.* N-*Dichlorofluoromethylthio-*N',N'-*dimethyl-*N-*phenylsulfamide. Euparen*†. *Elvaron*

[1085-98-9]

$Cl_2CF\text{-}S\text{-}NPh\text{-}SO_2NMe_2$

$C_9H_{11}Cl_2FN_2O_2S_2$ M 333.2
Protective fungicide with some acaricidal effect. Powder. Prac. insol. H_2O, sl. sol. MeOH, sol. xylene. Mp 105-106°.

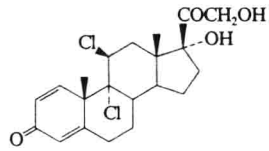
▶ LD_{50} (rat, orl) 500 mg/kg; LD_{50} (rat, skn) 1000 mg/kg. WO6475000.

U.K. Pat., 927 834, (1960); *CA*, **58**, 9093b.
Kuehle, E. *et al, Angew. Chem.*, 1964, **76**, 807 (*synth, activity*)
Suzuki, K. *et al, Agric. Biol. Chem.*, 1974, **38**, 1433 (*detn*)
Schupan, I. *et al, ACS Symp. Ser.*, 1981, **158**, 85 (*rev, metab*)
Pesticide Manual, 9th edn., 1991, No. 4150.
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DFL200.

Dichlorisone, INN D-0-03168

9,11β-Dichloro-17α,21-dihydroxypregna-1,4-diene-3,20-dione, 9CI. Sch 5350

[7008-26-6]



$C_{21}H_{26}Cl_2O_4$ M 413.3
Topical antipruritic, antiinflammatory, antiallergic agent. Cryst. (Me_2CO/hexane). Mp 238-241° dec. $[\alpha]_D^{20}$ +134 (Py).

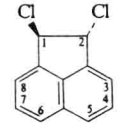
21-Ac: [79-61-8]. *Dichlorisone acetate. Astroderm. Diloderm. Diclasone*
$C_{23}H_{28}Cl_2O_5$ M 455.3 Antipruritic, antiinflammatory, antiallergic agent. Cryst. (Me_2CO/hexane). Mp 246-253° dec. $[\alpha]_D^{25}$ +162 (dioxan).

Robinson, C.H. *et al, J.A.C.S.*, 1959, **81**, 2191 (*uv, ir, synth, pharmacol*)
Bowers, A., *J.A.C.S.*, 1959, **81**, 4107 (*synth*)
Robinson, C.H. *et al, J.O.C.*, 1961, **26**, 2863 (*synth, uv*)
Shapiro, E. *et al, Steroids*, 1967, **9**, 143 (*esters*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 730.

1,2-Dichloroacenaphthene D-0-03169

1,2-Dichloro-1,2-dihydroacenaphthylene, 9CI

[5448-26-0]



(*1R*,2R**)-*form*

$C_{12}H_8Cl_2$ M 223.1

(*1R*,2R**)-*form* [54161-50-1]
(−)-trans-*form*
Cryst. (EtOH). Mp 102°. $[\alpha]_D^{22}$ −62.25 (c, 0.9 in Et_2O).

(*1RS,2RS*)-*form* [54075-01-3]
(±)-trans-*form*
Needles (EtOH aq.). Mp 67-68°. Spontaneously resolves on cryst.

(*1RS,2SR*)-*form* [49601-80-1]
cis(meso)-*form*
Plates (petrol), needles (EtOH). Mp 115°.

Campbell, B., *J.C.S.*, 1915, 918 (*synth*)
Cristol, S.J. *et al, J.A.C.S.*, 1956, **78**, 4939 (*synth*)
Bernardinelli, G. *et al, Acta Cryst. B*, 1974, **30**, 1594 (*cryst struct*)
Perucaud, M.-C. *et al, Bull. Soc. Chim. Fr.*, 1974, 1011.

3,5-Dichloroacenaphthene D-0-03170

3,5-Dichloro-1,2-dihydroacenaphthylene, 9CI

[27608-78-2]

$C_{12}H_8Cl_2$ M 223.1
Cryst. (EtOH). Mp 140-141°.

Petrenko, G.P. *et al, J. Org. Chem. USSR* (*Engl. Transl.*), 1970, **6**, 586.

5,6-Dichloroacenaphthene D-0-03171

5,6-Dichloro-1,2-dihydroacenaphthylene, 9CI. 4,5-Dichloroacenaphthene (obsol.)

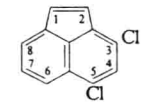
[4208-97-3]

$C_{12}H_8Cl_2$ M 223.1
Needles (hexane/C_6H_6). Mp 165.8-167.5°.

Morgan, G.T. *et al, J. Soc. Chem. Ind., London*, 1930, **49**, 413 (*synth*)
Miyamoto, H. *et al, Tet. Lett.*, 1986, **27**, 2011 (*synth*)

3,5-Dichloroacenaphthylene D-0-03172

[27608-79-3]



$C_{12}H_6Cl_2$ M 221.0
Yellow plates (C_6H_6). Mp 136°.

Petrenko, G.P. *et al, J. Org. Chem. USSR* (*Engl. Transl.*), 1970, **6**, 586 (*synth*)

5,6-Dichloroacenaphthylene D-0-03173

[7267-09-6]

$C_{12}H_6Cl_2$ M 221.0
Cryst. (C_6H_6). Mp 161.5-162.5°. Spar. sol. EtOH with mauve fluor.

Usachenko, V.G. *et al, J. Org. Chem. USSR* (*Engl. Transl.*), 1971, **7**, 1540 (*synth*)

Dichloroacetaldehyde, 9CI D-0-03174

Dichloroethanal

[79-02-7]

Cl_2CHCHO

$C_2H_2Cl_2O$ M 112.9
Liq. d^{25} 1.4113. Bp 90-91°. Polym. on standing or in presence of acid.

▶ Irritant. AB2710000.

Covalent hydrate: [16086-14-9]. *2,2-Dichloro-1,1-ethanediol*
$C_2H_4Cl_2O_2$ M 130.9 Crystallises from aq. solution of dichloroacetaldehyde. Cryst. Sol. H_2O. Mp 56-57° (43°). Bp 97° (118°).

Oxime: [75184-25-7]. *Dichloroacetaldoxime*
$C_2H_3Cl_2NO$ M 127.9 Liq. Bp_{17} 67-69°.
▶ Lachrymator.

Semicarbazone: Cryst. ($CHCl_3$). Mp 155° dec.

Di-Me acetal: [80944-06-5]. *1,1-Dichloro-2,2-dimethoxyethane, 9CI*
$C_4H_8Cl_2O_2$ M 159.0 Liq. Bp 166-168°.

Di-Et acetal: [619-33-0]. *1,1-Dichloro-2,2-diethoxyethane, 9CI*
$C_6H_{12}Cl_2O_2$ M 187.0 Liq. Bp 183-184°, Bp_{38} 107-108°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **1**, 361A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 222B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 292B (*ir*)
Kötz, A., *J. Prakt. Chem.*, 1914, **90**, 297 (*synth*)
U.K. Pat., 156 120, (1920); *CA*, **15**, 1728 (*synth*)
Routala, O. *et al*, *Ber.*, 1924, **57**, 252 (*oxime, synth*)
Lucazeau, G. *et al*, *J. Mol. Spectrosc.*, 1970, **35**, 214 (*uv*)
Lucazeau, G. *et al*, *J. Mol. Struct.*, 1970, **5**, 85 (*ir, Raman*)
Swietoslawski, J. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1976, **50**, 375 (*synth*)
Guengerich, F.P. *et al*, *Biochemistry*, 1983, **22**, 5482 (*synth, pmr*)
Wakasugi, T. *et al*, *Synth. Commun.*, 1993, **23**, 1289 (*synth*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DEM200.

Dichloroacetic acid, 9CI D-0-03175

Dichloroethanoic acid

[79-43-6]

$Cl_2CHCOOH$

$C_2H_2Cl_2O_2$ M 128.9
Has fungicidal props. Corrosive liq. d_4^{20} 1.563. Mp 5-6° (11°). Bp 194°, Bp_{20} 102°. n_D^{22} 1.4659.
▶ Fl. p. >66°. Corrosive and irritating to all tissues. LD_{50} (rbt, skn) 510 mg/kg. AG6125000.

Me ester: [116-54-1].
$C_3H_4Cl_2O_2$ M 142.9 Liq. Bp 143-144°.
▶ Skin, eye, and mucous membrane irritant. AG6625000.

Chloride: [79-36-7].
C_2HCl_3O M 147.3 Derivatisation reagent used in gc anal. of diethylstilbestrol. Liq. with acrid penetrating odour. Bp 108-111°.
▶ Corrosive to all tissues. AO6650000.

Amide: [683-72-7]. *Dichloroacetamide*
$C_2H_3Cl_2NO$ M 127.9 Constit. of the red alga *Marginisporum aberrans*. Preservative. Shows antimicrobial props. Cryst. Mp 98°. Bp_{745} 234°. Steam-volatile, subl.
▶ AB6475000.

Anhydride: [4124-30-5].
$C_4H_2Cl_4O_3$ M 239.8 Liq. Bp 215-216° dec., Bp_{35} 140°.
▶ Skin and eye irritant. AG6300000.

Nitrile: [3018-12-0]. *Dichlorocyanomethane*
C_2HCl_2N M 109.9 Liq. $d^{11.5}$ 1.374. Bp 113°.
▶ LD_{50} (rat, orl) 330 mg/kg. Exp. reprod. and teratogenic effects. AL8465000.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **1**, 792A, 1007C, 1223A, 1366C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 508B, 652C, 713C, 724B, 751D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 591C, 702D, 766B (*ir*)
Doughty, H.W., *J.A.C.S.*, 1931, **53**, 1594 (*synth, bibl*)
Liston, T.R. *et al*, *J.A.C.S.*, 1938, **60**, 1264 (*ester*)
Org. Synth., Coll. Vol., 2, 1943, 181 (*synth*)
Org. Synth., Coll. Vol., 3, 1955, 260 (*amide*)
Donoho, A.L. *et al*, *J. Assoc. Off. Anal. Chem.*, 1973, **56**, 785 (*use, chloride*)
Matsumura, K. *et al*, *Chem. Pharm. Bull.*, 1976, **24**, 912.
Fritz, H. *et al*, *Org. Magn. Reson.*, 1977, **9**, 108 (*cmr*)
Ohta, K. *et al*, *Phytochemistry*, 1977, **16**, 1085 (*isol, amide*)
Pellegata, R. *et al*, *Synthesis*, 1985, 517 (*amide*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1992, **16**, 115 (*use*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DEL000, DEM800, DEM825, DEN000, DEN400.
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, Cambridge, 1992, 409, 410.

2,2-Dichloroacetophenone D-0-03176

2,2-Dichloro-1-phenylethanone, 9CI. Phenacylidene chloride

[2648-61-5]

$PhCOCHCl_2$

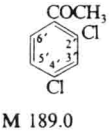
$C_8H_6Cl_2O$ M 189.0
Liq. or cryst. d 1.340. Mp 20-21.5°. Bp 249°, Bp_{11} 131-132°. With 2,4-Dinitrophenylhydrazine forms Phenylglyoxal bis(2,4-dinitrophenylhydrazone), red cryst., Mp 296° dec.
▶ Lachrymator, highly irritant. AM7175000.

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 20B (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., **2**, 22D (*nmr*)
Roberts, J.D. *et al*, *J.A.C.S.*, 1953, **75**, 4765.
Reed, S.R., *J.O.C.*, 1965, **30**, 2193.
Ficini, J. *et al*, *Bull. Soc. Chim. Fr.*, 1974, 1533 (*synth, ir, nmr*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DEN200.

2′,4′-Dichloroacetophenone D-0-03177

1-(2,4-Dichlorophenyl)ethanone, 9CI. 2,4-Dichlorophenyl methyl ketone

[2234-16-4]



$C_8H_6Cl_2O$ M 189.0
d_4^{22} 1.322. Mp 33-34°, Mp 42°. Bp_5 104-105°.

Oxime: [71516-67-1].
$C_8H_7Cl_2NO$ M 204.0 Needles (EtOH). Mp 152°, Mp 148°.

Semicarbazone: Needles (EtOH). Mp 208°.

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 29B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1250A (*ir*)
Aldrich Library of IR Spectra, 2nd Ed., 757B (*ir*)
Aldrich Library of NMR Spectra, **6**, 25B (*pmr*)
Aldrich Library of NMR Spectra, 2nd edn., **2**, 32B (*nmr*)
Kshatriya, K.C. *et al*, *J. Indian Chem. Soc.*, 1947, **24**, 373.
Lutz, R.E. *et al*, *J.O.C.*, 1947, **12**, 678.

2′,5′-Dichloroacetophenone D-0-03178

1-(2,5-Dichlorophenyl)ethanone, 9CI

[2476-37-1]

$C_8H_6Cl_2O$ M 189.0
Liq. or cryst. $d_4^{17.5}$ 1.352. Mp 14°. Bp 251°, Bp_3 102-104°.

Oxime: [71516-69-3].
$C_8H_7Cl_2NO$ M 204.0 Needles. Mp 127°, Mp 130°.

Semicarbazone: Needles (EtOH). Mp 202-203°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 839A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 30C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1251A (*ir*)
Aldrich Library of IR Spectra, 2nd Ed., 757G (*ir*)
Aldrich Library of NMR Spectra, **6**, 25D (*pmr*)
Kshatriya, K.C. *et al*, *J. Indian Chem. Soc.*, 1947, **24**, 373.
Lutz, R.E. *et al*, *J.O.C.*, 1947, **12**, 680.
Rajsner, M. *et al*, *Coll. Czech. Chem. Comm.*, 1978, **43**, 1276.

2′,6′-Dichloroacetophenone D-0-03179

1-(2,6-Dichlorophenyl)ethanone, 9CI

[2040-05-3]

$C_8H_6Cl_2O$ M 189.0
Mp 44°. Bp_1 73°.

Lock, G. *et al*, *Ber.*, 1937, **70**, 921.
Dhami, K.S., *Can. J. Chem.*, 1965, **43**, 479 (*synth, nmr*)

3′,4′-Dichloroacetophenone D-0-03180

1-(3,4-Dichlorophenyl)ethanone, 9CI

[2642-63-9]

$C_8H_6Cl_2O$ M 189.0
Needles (petrol or C_6H_6/petrol). Mp 76°. Bp_{13} 130-132°.

Oxime: [71516-68-2].
$C_8H_7Cl_2NO$ M 204.0 Mp 110°.

Semicarbazone: Needles (EtOH). Mp 250°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 839B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 29D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1250C (*ir*)
Aldrich Library of NMR Spectra, **6**, 25c (*pmr*)
Kshatriya, K.C. *et al*, *J. Indian Chem. Soc.*, 1947, **24**, 373 (*synth*)
Keneford, J.R. *et al*, *J.C.S.*, 1947, 227, 232 (*synth*)
Aw, C.T., *J.C.S. Perkin 2*, 1972, 1638 (*ir*)

3′,5′-Dichloroacetophenone D-0-03181

1-(3,5-Dichlorophenyl)ethanone, 9CI

[14401-72-0]

$C_8H_6Cl_2O$ M 189.0
Red oil solidifying on standing. Mp 26°. Bp_1 107-110°.

Oxime:
$C_8H_7Cl_2NO$ M 204.0 Mp 138°.

Lock, C.V. *et al*, *Ber.*, 1937, **70**, 922 (*synth*)
Lutz, R.E. *et al*, *J.O.C.*, 1947, **12**, 681 (*synth*)
Twine, C.J. *et al*, *J.O.C.*, 1974, **39**, 1290 (*ir, uv, ms*)

Dichloroacetylene, 8CI D-0-03182

Dichloroethyne, 9CI

[7572-29-4]

$ClC{\equiv}CCl$

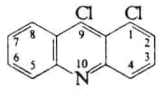
C_2Cl_2 M 94.9
Volatile liq. Mp −66° to −64.2°. Bp 33°.

▶ Heat-sensitive explosive. Ignites on contact with air. Adverse CNS effects. Reported human symptoms include disabling nausea and severe jaw pain. LC_{50} (mus, ihl) 19 ppm (6h exposure). Exp. carcinogen. OES: short-term 0.1 ppm. AP1080000.

Kloster-Jensen, E. *et al*, *Helv. Chim. Acta*, 1970, **53**, 2109 (*ms*)
Siegel, J. *et al*, *J.O.C.*, 1970, **35**, 3199 (*synth, bibl*)
Klaboe, P. *et al*, *Spectrochim. Acta A*, 1970, **26**, 1567 (*ir, Raman*)
Kloster-Jensen, E., *Tetrahedron*, 1971, **27**, 33 (*synth*)
Kende, A.S. *et al*, *Synthesis*, 1982, 455 (*synth*)
IARC Monog., 1986, **39**, 369; *Suppl.* 7, 62 (*rev, tox*)
Denis, J.-N. *et al*, *J.O.C.*, 1987, **52**, 3461 (*synth*)
Pielichowski, J. *et al*, *J. Prakt. Chem.*, 1989, **331**, 145 (*synth*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 3584.
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DEN600.
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworth, London and Boston, 1990, 0573.
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, Cambridge, 1992, 411.

1,9-Dichloroacridine, 9CI D-0-03183

[35547-69-4]



$C_{13}H_7Cl_2N$ M 248.1
Pale-yellow-green cryst. Mp 116-117°. Green fluor. soln. in AcOH/conc. H_2SO_4.

Lehmstedt, K. *et al*, *Ber.*, 1937, **70**, 838.
Wilkinson, J.H. *et al*, *J.C.S.*, 1948, 32.
Horowska, B. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1971, **45**, 1447; *CA*, **76**, 113040.

2,9-Dichloroacridine, 9CI D-0-03184

[1019-14-3]

$C_{13}H_7Cl_2N$ M 248.1
Cryst. (EtOH aq.). Mp 147°.

Ionescu, M. *et al*, *CA*, 1962, **57**, 12432.
Bogucka, M. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1966, **40**, 677; *CA*, **65**, 5440.
Fr. Pat., 1 530 413, (1970); *CA*, **72**, 5397.
Giri, S. *et al*, *Indian J. Chem., Sect. B*, 1978, **16**, 835.

3,9-Dichloroacridine, 9CI D-0-03185

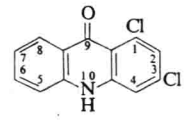
[35547-70-7]

$C_{13}H_7Cl_2N$ M 248.1
Pale-yellow cryst. (EtOH aq.). Mp 169-170°.

Lehmstedt, K. *et al*, *Ber.*, 1937, **70**, 838.
Wilkinson, J.H. *et al*, *J.C.S.*, 1948, 32.
Tanasescu, I. *et al*, *CA*, 1964, **61**, 1327.
Horowska, B. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1971, **45**, 1447; *CA*, **76**, 113040.

1,3-Dichloroacridone D-0-03186

1,3-Dichloro-9(10H)-acridinone, 9CI



$C_{13}H_7Cl_2NO$ M 264.1
Cryst. (Py). Mp 310°.

Nisbet, H.B. *et al*, *J.C.S.*, 1932, 2772; 1933, 1372.
Archer, S. *et al*, *J.A.C.S.*, 1954, **76**, 588.

1,4-Dichloroacridone D-0-03187

1,4-Dichloro-9(10H)-acridinone, 9CI

[56605-87-9]

$C_{13}H_7Cl_2NO$ M 264.1
Yellow needles. Mp 268°.

Nisbet, H.B., *J.C.S.*, 1933, 1372.

1,6-Dichloroacridone D-0-03188

1,6-Dichloro-9(10H)-acridinone, 9CI

$C_{13}H_7Cl_2NO$ M 264.1
Mp 416°. Blue fluor. in conc. H_2SO_4. Intense violet in EtOH → yellow-green with NaOH.

Tănăsescu, I. *et al*, *Bull. Soc. Chim. Fr.*, 1937, **4**, 245.

2,3-Dichloroacridone D-0-03189

2,3-Dichloro-9(10H)-acridinone, 9CI

$C_{13}H_7Cl_2NO$ M 264.1
Yellow cryst. Mp >360°. Sol. EtOH with blue fluor. → green on addn. of alkali.

Tănăsescu, I. *et al*, *Bull. Soc. Chim. Fr.*, 1939, **6**, 491.

2,4-Dichloroacridone D-0-03190

2,4-Dichloro-9(10H)-acridinone, 9CI

[35308-02-2]

$C_{13}H_7Cl_2NO$ M 264.1
Yellow needles (AcOH), cryst. (Py). Spar. sol. hot EtOH, insol. Et_2O, C_6H_6. Mp >360°. Blue fluor. sol. in conc. H_2SO_4. Light-yellow AcOH soln. with blue-viol. fluor.

Ullmann, F., *Annalen*, 1907, **355**, 339.

2,6-Dichloroacridone D-0-03191

2,6-Dichloro-9(10H)-acridinone, 9CI

$C_{13}H_7Cl_2NO$ M 264.1
Cryst. (AcOH). Mp 422-424°. Green fluor. soln. in conc. H_2SO_4.

Tănăsescu, I. *et al*, *Bull. Soc. Chim. Fr.*, 1936, **3**, 1753; 1937, **4**, 245.
Davis, R.B. *et al*, *J.O.C.*, 1960, **25**, 1884.

2,7-Dichloroacridone D-0-03192

2,7-Dichloro-9(10H)-acridinone, 9CI

[10352-33-7]

$C_{13}H_7Cl_2NO$ M 264.1
Yellow needles (AcOH). Mp 434°.

Ionescu, M. *et al*, *CA*, 1961, **55**, 533, 9402.
Ionescu, M. *et al*, *CA*, 1966, **65**, 20096.

3,6-Dichloroacridone D-0-03193

3,6-Dichloro-9(10H)-acridinone, 9CI

[5100-80-1]

$C_{13}H_7Cl_2NO$ M 264.1
Cryst. (Py aq.). Mp >360°.

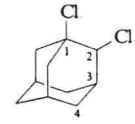
10-Hydroxy:
$C_{13}H_7Cl_2NO_2$ M 280.1 Mp 236-238°.

Spalding, D.P. *et al*, *J.A.C.S.*, 1946, **68**, 1596.
Braun, A., *Pol. J. Chem.* (*Rocz. Chem.*), 1962, **36**, 151; *CA*, **57**, 15071.

1,2-Dichloroadamantane, 8CI D-0-03194

1,2-Dichlorotricyclo[3.3.1.1^{3,7}]decane, 9CI

[29038-91-3]



$C_{10}H_{14}Cl_2$ M 205.1

(±)-form
Cryst. (MeOH). Mp 183-185° (178-180°) dec.

Cuddy, B.D. *et al*, *J.C.S.(C)*, 1971, 3173 (*synth, pmr, ms*)
Lenoir, R.G. *et al*, *J.O.C.*, 1971, **36**, 182 (*synth, ir, pmr, ms*)
Abdel-Sayed, A.N. *et al*, *Tetrahedron*, 1988, **44**, 1873, 1883 (*synth, pmr, cmr*)

1,3-Dichloroadamantane, 8CI D-0-03195

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

[16104-50-0]

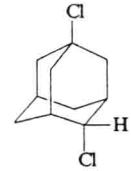
$C_{10}H_{14}Cl_2$ M 205.1
Cryst. (EtOH). Mp 132-134° (129-130°).

Harmill, H. *et al*, *Tetrahedron*, 1971, **27**, 4317 (*synth*)
Tolstikov, G.A. *et al*, *Tet. Lett.*, 1972, 3191 (*synth*)
Perkins, R.R. *et al*, *Org. Magn. Reson.*, 1976, **8**, 165 (*cmr*)
Barton, D.H.R. *et al*, *J.C.S. Perkin 1*, 1983, 445 (*synth*)
Becker, J.Y. *et al*, *J.O.C.*, 1988, **53**, 1744 (*synth, pmr*)

1,4-Dichloroadamantane D-0-03196

1,4-Dichlorotricyclo[3.3.1.1^{3,7}]decane, 9CI

[20098-15-1]



(1RS,4RS)-form

$C_{10}H_{14}Cl_2$ M 205.1

(1RS,4RS)-form [39646-69-0]
Mp 131.5-133.5°.

(1RS,4SR)-form [39646-70-3]
Mp 157-159°.

Geluk, H.W. *et al*, *Tetrahedron*, 1968, **24**, 5369.
Yang, K.H. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 2217.

,2-Dichloroadamantane, 8CI D-0-03197

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

[7419-57-0]

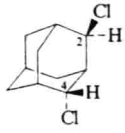
$C_{10}H_{14}Cl_2$ M 205.1
Cryst. (petrol). Mp 203-204°.

Cuddy, B.D. *et al*, *J.C.S. Perkin 1*, 1972, 2701 (*synth*)
Duddeck, H. *et al*, *Org. Magn. Reson.*, 1976, **8**, 593 (*cmr*)
Archibald, T.G. *et al*, *J.O.C.*, 1988, **53**, 4645 (*synth*)

2,4-Dichloroadamantane, 8CI D-0-03198

2,4-Dichlorotricyclo[3.3.1.1^{3,7}]decane, 9CI

[34341-84-9]



(*2RS,4RS*)-*form*

$C_{10}H_{14}Cl_2$ M 205.1

(***2RS,4RS*)-*form*** [21940-10-3]
Mp 170-175°.

(***2RS,4SR*)-*form*** [21939-92-4]
Mp 120-122°.

[19087-15-1, 19288-31-4]

Van Deursen, F.W. *et al*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1968, **87**, 1243 (*pmr*)
Udding, A.C. *et al*, *Tet. Lett.*, 1968, 1345 (*synth*)
Van Deursen, F.W. *et al*, *Tetrahedron*, 1971, **27**, 4593 (*pmr*)
Duddek, H., *Tetrahedron*, 1978, **34**, 247 (*cmr*)

4-[(Dichloroamino)sulfonyl] benzoic acid, 9CI D-0-03199

Benzoic acid p-N-*dichlorosulfonamide*. N-*Dichloro-4-sulfonamidobenzoic acid*. p-(*Dichlorosulfamoyl)benzoic acid*. ***Halazone*, INN, USAN.** *Alazone. Cloritines. Pantocid. Zeptabs*

[80-13-7]

$C_7H_5Cl_2NO_4S$ M 270.0
Germicide. Used to sterilise drinking water, prob. by generation of HOCl. Cryst. with chlorine odour. Mp 196° dec., Mp 213°. Coml. halazone also contains the corresponding monochloro compd.

▶ DG8050000.

Na salt: [5698-56-6]. *Aseptamide. Cavosept. Gynamide. Pantosept. Phenochlorium. Sulfochloramin. Theragynes*

Et ester:
$C_9H_9Cl_2NO_4S$ M 298.1 Mp 80°.

Victorin, K. *et al*, *J. Hyg.*, 1972, **70**, 313 (*use*)
Saljoughian, M. *et al*, *Monatsh. Chem.*, 1986, **117**, 553 (*synth, bibl*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, London, 1993, 796.
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, HAF000.

2,3-Dichloroaniline, 8CI D-0-03200

2,3-Dichlorobenzenamine, 9CI

[608-27-5]

$C_6H_5Cl_2N$ M 162.0
Needles (petrol). Mp 24°. Bp 252°. pK_{a1} 1.76 (25°, H_2O), pK_{a1} 22.13 (DMSO aq.).

▶ Fl. p. >110°.

N-*Ac:* [23068-36-2]. *2,3-Dichloroacetanilide*
$C_8H_7Cl_2NO$ M 204.0 Needles (C_6H_6). Mp 157°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 492A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1215A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1133D (*ir*)
Aldrich Library of IR Spectra, 2nd Ed., 641G (*ir*)
Aldrich Library of NMR Spectra, **5**, 62D (*pmr*)
Sadtler Standard C-13 NMR Spectra, 1118 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 6233 (*uv*)
Beilstein, F. *et al*, *Annalen*, 1879, **196**, 214 (*synth*)

2,4-Dichloroaniline, 8CI D-0-03201

2,4-Dichlorobenzenamine, 9CI

[554-00-7]

$C_6H_5Cl_2N$ M 162.0
Needles (EtOH). Mp 63°. Bp 245°. pK_{a1} 2.00 (25°, H_2O), pK_{a1} 22.6 (DMSO aq.).

▶ LD_{50} (rat, orl) 1600 mg/kg. BX2600000.

N-*Ac:* [6975-29-7]. *2,4-Dichloroacetanilide*
$C_8H_7Cl_2NO$ M 204.0 Prisms (EtOH). Mp 147°.

N-*Benzoyl:* [10286-76-7].
$C_{13}H_9Cl_2NO$ M 266.1 Needles (EtOH). Mp 117°.

N-*Me:* [35113-88-3].
$C_7H_7Cl_2N$ M 176.0 Mp 25°.

N-*Di-Me:* [35113-90-7].
$C_8H_9Cl_2N$ M 190.0 Liq. Bp 234°, Bp_2 92-95°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 504C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1219D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1140A (*ir*)
Aldrich Library of IR Spectra, 2nd Ed., 644F (*ir*)
Aldrich Library of NMR Spectra, **5**, 68C (*pmr*)
Sadtler Standard C-13 NMR Spectra, 3564 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 16957 (*uv*)
Beilstein, F. *et al*, *Annalen*, 1876, **182**, 94 (*synth, deriv*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th edn., Van Nostrand Reinhold, 1979, 557.

2,5-Dichloroaniline, 8CI D-0-03202

2,5-Dichlorobenzenamine, 9CI

[95-82-9]

$C_6H_5Cl_2N$ M 162.0
Needles (petrol). Mp 50°. Bp 251°, Bp_{11} 107°. pK_{a1} 1.53 (25°), pK_{a1} 22.71 (25°, DMSO aq.).

▶ LD_{50} (rat, orl) 2900 mg/kg. BX2610000.

Hydrochloride: [33663-41-1].
Mp 191-192°.

N-*Ac:* [2621-62-7]. *2,5-Dichloroacetanilide*
$C_8H_7Cl_2NO$ M 204.0 Cryst. (EtOH). Mp 133°.

▶ AE1965000.

N-*Benzoyl:* [6626-75-1].
$C_{13}H_9Cl_2NO$ M 266.1 Needles (EtOH). Mp 122°.

▶ CV3620000.

N-*Me:* [10224-70-1].
$C_7H_7Cl_2N$ M 176.0 Oil.

N-*Di-Me:* [75560-63-3].
$C_8H_9Cl_2N$ M 190.0 Bp_{20} 122.5°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 505A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1220A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1140B (*ir*)
Aldrich Library of IR Spectra, 2nd Ed., 644G (*ir*)
Aldrich Library of NMR Spectra, **5**, 69A (*pmr*)
Sadtler Standard C-13 NMR Spectra, 4672 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 253 (*uv*)
Winans, C.F., *J.A.C.S.*, 1939, **61**, 3564 (*synth*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DEO400.

2,6-Dichloroaniline, 8CI D-0-03203

2,6-Dichlorobenzenamine, 9CI

[608-31-1]

$C_6H_5Cl_2N$ M 162.0
Needles (EtOH aq.). Mp 39-40°. pK_{a1} 0.42 (25°, H_2O), pK_{a1} 23.64 (25°, DMSO aq.).

N-*Ac:* [17700-54-8]. *2,6-Dichloroacetanilide*
$C_8H_7Cl_2NO$ M 204.0 Needles (AcOH aq.). Mp 175°.

▶ LD_{50} (mus, orl) 418 mg/kg. AE1970000.

N-*Benzoyl:* [10286-88-1].
$C_{13}H_9Cl_2NO$ M 266.1 Mp 158-159°.

N-*Me:*
$C_7H_7Cl_2N$ M 176.0 Bp 128-130°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 491C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1214D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1133C (*ir*)
Aldrich Library of IR Spectra, 2nd Ed., 641F (*ir*)
Aldrich Library of NMR Spectra, **5**, 62B (*pmr*)
Sadtler Standard C-13 NMR Spectra, 6788 (*cmr*)
Org. Synth., Coll. Vol., 3, 1955, 262 (*synth*)
Ishii, H. *et al*, *Chem. Pharm. Bull.*, 1990, **38**, 597 (*N*-Me)

3,4-Dichloroaniline, 8CI D-0-03204

3,4-Dichlorobenzenamine, 9CI

[95-76-1]

$C_6H_5Cl_2N$ M 162.0
Needles (petrol). Mp 72°. Bp 272°, Bp_{15} 144-146°. pK_{a1} 2.96 (25°, H_2O), pK_{a1} 25.07 (25°, DMSO aq.).

▶ Fl. p. 166° (oc). Severe eye and skin irritant. LD_{50} (rat, orl) 648 mg/kg. LD_{50} (cat, skn) 700 mg/kg. BX2625000.

N-*Ac:* [2150-93-8]. *3,4-Dichloroacetanilide*
$C_8H_7Cl_2NO$ M 204.0 Cryst. (EtOH aq.). Mp 122.5°.

N-*Propanoyl:* [709-98-8]. N-*(3,4-Dichlorophenyl)propanamide, 9CI. 3',4'-Dichloropropionanilide. Propanil, BSI, ISO, WSSA. Stam. Surcopur. Rogue. DCPA, JMAF. Propanide*
Contact herbicide. Solid, tech. grade freq. liq. Mp 92-93°.
▶ Mod. high toxicity. LD_{50} (rat, orl) 560 mg/kg. UE4900000.

N-*Benzoyl:* [10286-75-6].
$C_{13}H_9Cl_2NO$ M 266.1 Cryst. (EtOH). Mp 143-144°.

N,N-*Di-Me:* [58566-66-8].
$C_8H_9Cl_2N$ M 190.0 Needles (HCl aq.). Mp 38-39°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 504B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1219C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1139D (*ir*)
Aldrich Library of IR Spectra, 2nd Ed., 644E (*ir*)
Aldrich Library of NMR Spectra, **5**, 68A (*pmr*)
Sadtler Standard C-13 NMR Spectra, 6238 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 1794 (*uv*)
Hodgson, H.H. *et al*, *J.C.S.*, 1929, 2917 (*synth*)
Ger. Pat., 1 039 779, (1958); *CA*, **54**, 20060i (*Propanil*)
Stephenson, G.R. *et al*, *J. Agric. Food Chem.*, 1979, **27**, 543 (*Propanil*)
Cabras, P. *et al*, *J. Chromatogr.*, 1982, **234**, 249 (*Propanil*)
Lay, J.O. *et al*, *Biomed. Environ. Mass Spectrom.*, 1986, **13**, 495 (*Propanil*)
Pesticide Manual, 9th edn., 1991, No. 10120 (*Propanil*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A343 (*Propanil*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DEO300, DGI000.

3,5-Dichloroaniline, 8CI D-0-03205

3,5-Dichlorobenzenamine, 9CI

[626-43-7]

$C_6H_5Cl_2N$ M 162.0
Needles. Mp 52-53°. $Bp_{740.6}$ 259-260°. pK_{a1} 2.38 (25°, H_2O), pK_{a1} 24.05 (25°, DMSO aq.).

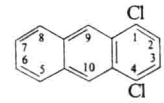
N-*Di-Me:* [35114-04-6].
$C_8H_9Cl_2N$ M 190.0 Platelets (MeOH). Mp 55°. Bp_{740} 264°.

N-*Ac:* [31592-84-4]. *3,5-Dichloroacetanilide*
$C_8H_7Cl_2NO$ M 204.0 Cryst. (EtOH). Mp 191°.

N-*Benzoyl:*
$C_{13}H_9Cl_2NO$ M 266.1 Cryst. (EtOH). Mp 149°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 520B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1229B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1147C (*ir*)
Aldrich Library of IR Spectra, 2nd Ed., 648C (*ir*)
Aldrich Library of NMR Spectra, **5**, 76C (*pmr*)
Sadtler Standard C-13 NMR Spectra, 6292 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 6259 (*uv*)
Dyson, G.M. *et al*, *J.C.S.*, 1926, 3041 (*synth*)

1,4-Dichloroanthracene D-0-03206



$C_{14}H_8Cl_2$ M 247.1
Yellow cryst. (butanone). Mp 180°.

Barnett, E. de B. *et al*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1926, **45**, 558 (*synth*)

1,5-Dichloroanthracene D-0-03207

[6406-96-8]

$C_{14}H_8Cl_2$ M 247.1
Yellow needles (butanol). Mp 187°.

Schilling, H., *Ber.*, 1913, **46**, 1066.
Bergmann, W.J., *J.A.C.S.*, 1938, **60**, 1804.
Porter, G. *et al*, *Proc. R. Soc. London, A*, 1964, **277**, 437.

1,6-Dichloroanthracene D-0-03208

$C_{14}H_8Cl_2$ M 247.1
Golden plates (AcOH). Mp 149-150°.

Goldberg, A.A., *J.C.S.*, 1931, 1781 (*synth*)

1,7-Dichloroanthracene D-0-03209

$C_{14}H_8Cl_2$ M 247.1
Yellow needles (AcOH). Mp 160-161°.

Goldberg, A.A., *J.C.S.*, 1931, 1781 (*synth*)

1,8-Dichloroanthracene D-0-03210

[14381-66-9]

$C_{14}H_8Cl_2$ M 247.1
Pale-yellow needles (2-propanol). Mp 156.5-158°.

Schilling, H., *Ber.*, 1913, **46**, 1066.
Bergmann, W.J., *J.A.C.S.*, 1938, **60**, 1804.
Stock, L.M. *et al*, *J.A.C.S.*, 1972, **94**, 3080 (*synth*)
House, H.O. *et al*, *J.O.C.*, 1973, **38**, 1167; 1986, **51**, 921 (*synth, nmr*)
Guilard, R. *et al*, *J.A.C.S.*, 1992, **114**, 9877 (***synth***, *pmr*)

1,9-Dichloroanthracene D-0-03211

$C_{14}H_8Cl_2$ M 247.1
Yellow needles. Mp 127-128°.

Liebermann, C. *et al*, *Ber.*, 1914, **47**, 1011 (*synth*)

1,10-Dichloroanthracene, 9CI D-0-03212

[22980-71-8]

$C_{14}H_8Cl_2$ M 247.1
Cryst. (EtOH). Mp 129°.

Clar, E. *et al*, *Bull. Soc. Chim. Fr.*, 1950, 433.
Heller, E. *et al*, *Isr. J. Chem.*, 1971, **9**, 449 (*synth, cryst struct*)

2,3-Dichloroanthracene, 9CI D-0-03213

[613-07-0]

$C_{14}H_8Cl_2$ M 247.1
Pale-yellow leaflets. Sol. AcOH, EtOAc, hot EtOH, spar. sol. $CHCl_3$. Mp 261° (255°). Subl. with part. dec.

Kircher, G., *Annalen*, 1887, **238**, 347.
Barnett, M. *et al*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1926, **45**, 561.
Cristol, S.J. *et al*, *J.O.C.*, 1975, **40**, 2171 (*synth*)

2,6-Dichloroanthracene, 9CI D-0-03214

[26154-35-8]

$C_{14}H_8Cl_2$ M 247.1
Cryst. (xylene), yellow plates (C_6H_6). Mp 273-274°. Bp_3 200° subl.

Hachiro, H. *et al*, *Nippon Kagaku Kaishi*, 1949, **52**, 198 (*synth*)
Agosta, W.C. *et al*, *J.O.C.*, 1970, **35**, 3856 (*synth*)
Hagishita, S. *et al*, *Tetrahedron*, 1972, **28**, 1435 (*synth*)

9,10-Dichloroanthracene D-0-03215

ms-*Dichloroanthracene*

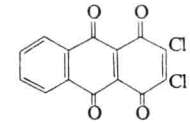
[605-48-1]

$C_{14}H_8Cl_2$ M 247.1
Yellow needles (CCl_4). Sol. C_6H_6, spar. sol. Et_2O, EtOH. Mp 212-212.5°. Oxidn. → anthraquinone.

Aldrich Library of FT-IR Spectra, 1st edn., **1**, 1032A (*ir*)
Ninaev, F., *CA*, 1931, **25**, 1252.
Karolina, P., *Pol. J. Chem. (Rocz. Chem.)*, 1974, **48**, 1453 (*synth*)
Sharpless, N.E. *et al*, *Org. Magn. Reson.*, 1974, **6**, 115 (*nmr*)
Stoesser, R. *et al*, *J. Prakt. Chem.*, 1975, **317**, 591 (*nmr*)
Trotter, J., *Acta Cryst. C*, 1986, **42**, 862 (*cryst struct*)

2,3-Dichloro-1,4,9,10-anthracenetetrone, 9CI D-0-03216

[109141-98-2]



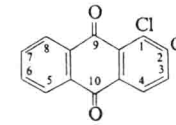
$C_{14}H_4Cl_2O_4$ M 307.0
Cryst. ($PhNO_2/CS_2$). Mp 224-226°.

Cano, P. *et al*, *J.C.S. Perkin 1*, 1986, 1923 (*synth, pmr*)

1,2-Dichloroanthraquinone, 8CI D-0-03217

1,2-Dichloro-9,10-anthracenedione, 9CI. 1,2-Dichloro-9,10-dihydro-9,10-dioxoanthracene

[1594-46-3]



$C_{14}H_6Cl_2O_2$ M 277.1
Dye intermediate. Yellow needles (AcOH). Mp 203° (196.5°).

Fierz-David, H.E., *J.A.C.S.*, 1927, **49**, 2334 (*synth*)
Goldberg, A.A., *J.C.S.*, 1931, 1771 (*synth*)
Volkov, A.F. *et al*, *J. Struct. Chem. (Engl. Transl.)*, 1975, **16**, 296 (*cryst struct*)

1,3-Dichloroanthraquinone, 8CI D-0-03218

1,3-Dichloro-9,10-anthracenedione, 9CI. 1,3-Dichloro-9,10-dihydro-9,10-dioxoanthracene

[602-73-3]

$C_{14}H_6Cl_2O_2$ M 277.1

Dye intermediate. Yellow needles (AcOH). Mp 209-210°.

Goldberg, A.A., *J.C.S.*, 1931, 2829 (*synth*)
Volkov, A.F. *et al*, *J. Struct. Chem.* (*Engl. Transl.*), 1975, **16**, 296 (*cryst struct*)

1,4-Dichloroanthraquinone, D-0-03219

8CI

1,4-Dichloro-9,10-anthracenedione, *9CI. 1,4-Dichloro-9,10-dihydro-9,10-dioxoanthracene*

[602-25-5]

$C_{14}H_6Cl_2O_2$ M 277.1
Dye intermediate. Orange-yellow cryst. (AcOH). Mp 187.5°.

Phillips, J., *J.A.C.S.*, 1926, **48**, 3198 (*synth*)
Nepras, M. *et al*, *Coll. Czech. Chem. Comm.*, 1963, **28**, 2706 (*uv*, *isol*)
Volkov, A.F. *et al*, *J. Struct. Chem.* (*Engl. Transl.*), 1975, **16**, 296 (*cryst struct*)

1,5-Dichloroanthraquinone, D-0-03220

8CI

1,5-Dichloro-9,10-anthracenedione, *9CI. 1,5-Dichloro-9,10-dihydro-9,10-dioxoanthracene*

[82-46-2]

$C_{14}H_6Cl_2O_2$ M 277.1
Dye intermediate. Yellow needles (AcOH). Mp 245°.

▶ Eye irritant. CB6495000.

(E,E)-*Dioxime:*
$C_{14}H_8Cl_2N_2O_2$ M 307.1 Mp 250° dec.
(E,Z)-*Dioxime:*
$C_{14}H_8Cl_2N_2O_2$ M 307.1 Mp 267° dec.
(Z,Z)-*Dioxime:*
$C_{14}H_8Cl_2N_2O_2$ M 307.1 Mp 207°.

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 86B (*ir*)
Fierz-David, H.E., *Helv. Chim. Acta*, 1927, **10**, 197 (*synth*)
Goldberg, A.A., *J.C.S.*, 1931, 1771 (*synth*)
Rydon, H.N. *et al*, *J.C.S.*, 1957, 1900.
Nepras, M. *et al*, *Coll. Czech. Chem. Comm.*, 1963, **28**, 2706 (*uv*)
Volkov, A.F. *et al*, *J. Struct. Chem.* (*Engl. Transl.*), 1975, **16**, 296 (*cryst struct*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DEO700.

1,6-Dichloroanthraquinone, D-0-03221

8CI

1,6-Dichloro-9,10-anthracenedione, *9CI. 1,6-Dichloro-9,10-dihydro-9,10-dioxoanthracene*

[727-51-5]

$C_{14}H_6Cl_2O_2$ M 277.1
Dye intermediate. Pale-yellow needles (AcOH). Mp 203-204°.

Fierz-David, H.E., *Helv. Chim. Acta*, 1927, **10**, 197 (*synth*)
Goldberg, A.A., *J.C.S.*, 1931, 1771 (*synth*)
Nepras, M. *et al*, *Coll. Czech. Chem. Comm.*, 1963, **28**, 2706 (*uv*)
Volkov, A.F. *et al*, *J. Struct. Chem.* (*Engl. Transl.*), 1975, **16**, 296 (*cryst struct*)

1,7-Dichloroanthraquinone, D-0-03222

8CI

1,7-Dichloro-9,10-anthracenedione, *9CI. 1,7-Dichloro-9,10-dihydro-9,10-dioxoanthracene*

[1594-69-0]

$C_{14}H_6Cl_2O_2$ M 277.1
Dye intermediate. Yellow needles (AcOH). Mp 213-214°.

Fierz-David, H.E., *Helv. Chim. Acta*, 1927, **10**, 197 (*synth*)
Goldberg, A.A., *J.C.S.*, 1931, 1771 (*synth*)
Nepras, M. *et al*, *Coll. Czech. Chem. Comm.*, 1963, **28**, 2706 (*uv*, *isol*)

1,8-Dichloroanthraquinone, D-0-03223

8CI

1,8-Dichloro-9,10-anthracenedione, *9CI. 1,8-Dichloro-9,10-dihydro-9,10-dioxoanthracene*

[82-43-9]

$C_{14}H_6Cl_2O_2$ M 277.1
Dye intermediate. Pale-yellow needles ($PhNO_2$). Mp 201-202°.

▶ Eye irritant. CB6496000.

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 86A (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., **2**, 90C (*nmr*)
U.S. Pat., 1 761 620, (1930); *CA*, **24**, 3520 (*synth*)
Goldberg, A.A., *J.C.S.*, 1931, 177 (*synth*)
Nepras, M. *et al*, *Coll. Czech. Chem. Comm.*, 1963, **28**, 2706 (*uv*)
Volkov, A.F. *et al*, *J. Struct. Chem.* (*Engl. Transl.*), 1975, **16**, 296 (*cryst struct*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DEO750.

2,3-Dichloroanthraquinone, D-0-03224

8CI

2,3-Dichloro-9,10-anthracenedione, *9CI. 2,3-Dichloro-9,10-dihydro-9,10-dioxoanthracene*

[84-45-7]

$C_{14}H_6Cl_2O_2$ M 277.1
Dye intermediate. Yellow needles (AcOH). Spar. sol. AcOH. Mp 267° (258-259°).

Phillips, M., *J.A.C.S.*, 1927, **49**, 473 (*synth*)
Goldberg, A.A., *J.C.S.*, 1931, 1771 (*synth*)
Nepras, M. *et al*, *Coll. Czech. Chem. Comm.*, 1963, **28**, 2706 (*uv*, *isol*)
Volkov, A.F., *J. Struct. Chem.* (*Engl. Transl.*), 1975, **16**, 296 (*cryst struct*)

2,6-Dichloroanthraquinone, D-0-03225

8CI

2,6-Dichloro-9,10-anthracenedione, *9CI. 2,6-Dichloro-9,10-dihydro-9,10-dioxoanthracene*

[605-40-3]

$C_{14}H_6Cl_2O_2$ M 277.1
Dye intermediate. Pale-yellow leaflets (PhCl). Mp 282°, Mp 302°.

Fierz-David, H.E., *Helv. Chim. Acta*, 1927, **10**, 225 (*synth*)
Nepras, M. *et al*, *Coll. Czech. Chem. Comm.*, 1963, **28**, 2706 (*uv*)
Volkov, A.F. *et al*, *J. Struct. Chem.* (*Engl. Transl.*), 1975, **16**, 296 (*cryst struct*)

2,7-Dichloroanthraquinone, D-0-03226

8CI

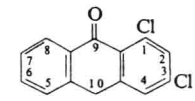
2,7-Dichloro-9,10-anthracenedione, *9CI. 2,7-Dichloro-9,10-dihydro-9,10-dioxoanthracene*

[605-43-6]

$C_{14}H_6Cl_2O_2$ M 277.1
Dye intermediate. Yellow needles (anisole). Mp 231°.

Fierz-David, H.E., *Helv. Chim. Acta*, 1927, **10**, 227 (*synth*)
Nepras, M. *et al*, *Coll. Czech. Chem. Comm.*, 1963, **28**, 2706 (*uv*)
Volkov, A.F. *et al*, *J. Struct. Chem.* (*Engl. Transl.*), 1975, **16**, 296 (*cryst struct*)

1,3-Dichloroanthrone D-0-03227



$C_{14}H_8Cl_2O$ M 263.1
Cryst. (AcOH or C_6H_6). Mp 194°.

Barnett, E. de B. *et al*, *Ber.*, 1933, **66**, 1876.

1,4-Dichloroanthrone D-0-03228

$C_{14}H_8Cl_2O$ M 263.1
Yellow needles (C_6H_6), cryst. (EtOH).

Eckert, A. *et al*, *Monatsh. Chem.*, 1918, **39**, 839.
Barnett, E. de B. *et al*, *Ber.*, 1929, **62**, 1971.

1,5-Dichloroanthrone D-0-03229

$C_{14}H_8Cl_2O$ M 263.1
Yellow needles (C_6H_6). Mp 192°.

Barnett, E. de B. *et al*, *J.C.S.*, 1923, **123**, 2549.

1,8-Dichloroanthrone D-0-03230

$C_{14}H_8Cl_2O$ M 263.1
Yellow needles (EtOH). Mp 167°.

Eckert, A. *et al*, *Monatsh. Chem.*, 1918, **39**, 839.
Barnett, E. de B. *et al*, *J.C.S.*, 1923, **123**, 2549; 1932, 506.

2,3-Dichloroanthrone D-0-03231

$C_{14}H_8Cl_2O$ M 263.1
Yellow cryst. (AcOH). Mp 202°.

Barnett, E. de B. *et al*, *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1926, **45**, 559.

2,4-Dichloroanthrone D-0-03232

$C_{14}H_8Cl_2O$ M 263.1
Yellow cryst. Mp 161°.

Barnett, E. de B. *et al*, *Ber.*, 1933, **66**, 1876.

4,5-Dichloroanthrone D-0-03233

$C_{14}H_8Cl_2O$ M 263.1
Needles (Me_2CO). Mp 198°.

Barnett, E. de B. *et al*, *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1926, **45**, 68.

4,10-Dichloroanthrone D-0-03234

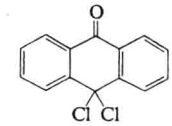
$C_{14}H_8Cl_2O$ M 263.1
Pale-yellow cryst. (petrol). Mp 127-128°.

Matthews, M.A., *J.C.S.*, 1926, 236.

10,10-Dichloroanthrone D-0-03235

10,10-Dichloro-9(10H)-anthracenone, *9CI. Anthraquinone dichloride*

[38032-82-5]



$C_{14}H_8Cl_2O$ M 263.1
Prisms (C_6H_6 or EtOH aq.). Mp 132-134°. Hydrol. by H_2O to Anthraquinone.

Kozlov, V.V., *Zh. Obshch. Khim.*, 1948, **18**, 757 (*synth*)
Etienne, A. *et al*, *Bull. Soc. Chim. Fr.*, 1951, 733 (*synth*)

Dichloroarsinoacetic acid D-0-03236

Carboxymethyldichloroarsine

Cl_2AsCH_2COOH

$C_2H_3AsCl_2O_2$ M 204.8
Synth. from $HOOCCH_2AsO_3H_2$ and PCl_3. White cryst. (CCl_4 or C_6H_6). Mp 122°.

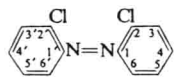
Me ester: Methyl dichloroarsinoacetate
$C_3H_5AsCl_2O_2$ M 218.8 Liq. Bp_5 78°.

Steinkopf, W. *et al*, *Ber.*, 1928, **61**, 675 (*synth*)
Hamer, D. *et al*, *J.C.S.*, 1961, 1398 (*synth, ir*)

2,2′-Dichloroazobenzene D-0-03237

Bis(2-chlorophenyl)diazene, 9CI

[7334-33-0]



$C_{12}H_8Cl_2N_2$ M 251.1

N^1-*Oxide:* [13556-84-8]. *2,2′-Dichloroazoxybenzene. Bis(2-chlorophenyl) diazine 1-oxide, 9CI*
$C_{12}H_8Cl_2N_2O$ M 267.1 Yellow needles (EtOH or cyclohexane). Mp 57-58° (53-54°).

(*E*)-*form* [49795-06-4]
Red plates (C_6H_6/petrol). Mp 138-139°.

(*Z*)-*form* [63213-02-5]
Mp 91-92°.

Zechmeister, L. *et al*, *Annalen*, 1929, **468**, 130.
Gore, P.H. *et al*, *J.A.C.S.*, 1956, **78**, 2160 (*oxide*)
Katsumi, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1967, **40**, 1538.
Sekiya, M. *et al*, *Chem. Pharm. Bull.*, 1970, **18**, 2146 (*oxide*)
Yamamoto, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1971, **44**, 2018 (*uv*)
Fahey, D.R., *J. Organomet. Chem.*, 1971, **27**, 283 (*ir, nmr, ms*)
Komeyama, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 2606 (*cryst struct*)
Rondestredt, C.S. *et al*, *Synthesis*, 1977, **12**, 850 (*oxide*)
Hyatt, J.A., *Tet. Lett.*, 1977, 141.
Alper, H., *J. Organomet. Chem.*, 1978, **144**, C18.

2,4-Dichloroazobenzene D-0-03238

(2,4-Dichlorophenyl)phenyldiazene, 9CI

$C_{12}H_8Cl_2N_2$ M 251.1
Orange cryst. (Et_2O or EtOH). Mp 107°.

Stieglitz, J. *et al*, *J.A.C.S.*, 1916, **38**, 1748.
Lewis, G.E. *et al*, *Aust. J. Chem.*, 1968, **21**, 1601.

2,4′-Dichloroazobenzene D-0-03239

(2-Chlorophenyl)(4-chlorophenyl)diazene, 9CI

[20039-10-5]

$C_{12}H_8Cl_2N_2$ M 251.1
Orange needles (petrol). Mp 112-113°.

Lewis, G.E. *et al*, *Aust. J. Chem.*, 1968, **21**, 1601.

2,5-Dichloroazobenzene D-0-03240

(2,5-Dichlorophenyl)phenyldiazene, 9CI

$C_{12}H_8Cl_2N_2$ M 251.1
Red solid (AcOH aq.). Mp 64°.

de Crauw, Th., *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1931, **50**, 777.

3,3′-Dichloroazobenzene D-0-03241

Bis(3-chlorophenyl)diazene, 9CI

[15426-14-9]

$C_{12}H_8Cl_2N_2$ M 251.1
Orange needles (EtOH or C_6H_6 or C_6H_6/AcOH). Mp 103-104°.

N-*Oxide:* [139-24-2]. *3,3′-Dichloroazoxybenzene. Bis(3-chlorophenyl) diazene 1-oxide, 9CI*
$C_{12}H_8Cl_2N_2O$ M 267.1 Pale-yellow needles (EtOH). Mp 96-97°.

Zechmeister, L. *et al*, *Annalen*, 1929, **468**, 129 (*oxide*)
Lock, G. *et al*, *Ber.*, 1936, **69**, 2666, 2669.
Gore, P.H. *et al*, *J.A.C.S.*, 1956, **78**, 2160 (*oxide*)
Katsumi, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1967, **40**, 1538 (*synth*)
Linke, H.A.B. *et al*, *Z. Naturforsch., B*, 1969, **24**, 997 (*uv, ir*)
Sekiya, M. *et al*, *Chem. Pharm. Bull.*, 1970, **18**, 2146 (*oxide*)
Alper, H. *et al*, *J. Organomet. Chem.*, 1978, **144**, C18 (*synth*)

4,4′-Dichloroazobenzene D-0-03242

Bis(4-chlorophenyl)diazene, 9CI

[1602-00-2]

$C_{12}H_8Cl_2N_2$ M 251.1

▶ CN2330000.

N-*Oxide:* [614-26-6]. *4,4′-Dichloroazoxybenzene. Bis(4-chlorophenyl) diazene 1-oxide, 9CI*
$C_{12}H_8Cl_2N_2O$ M 267.1 Yellow needles (EtOH). Mp 158° (154-155°).

▶ CO4050000.

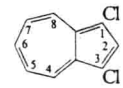
(*E*)-*form* [21650-51-1]
Pale-yellow needles (Me_2CO). Mp 189°.

(*Z*)-*form* [30926-04-6]
Needles (Me_2CO). Mp 66-68°, Mp 129-130°.

Aldrich Library of IR Spectra, 2nd Ed.,, 1262B (*ir*)
Zechmeister, L., *Annalen*, 1929, **468**, 129 (*oxide*)
Gore, P.H. *et al*, *J.A.C.S.*, 1956, **78**, 2160 (*oxide*)
Katsumi, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1967, **40**, 1538.
Hope, H. *et al*, *Acta Cryst. B*, 1969, **25**, 1849 (*cryst struct*)
Linke, H.A.B. *et al*, *Z. Naturforsch., B*, 1969, **24**, 997 (*uv, ir*)
Sekiya, M. *et al*, *Chem. Pharm. Bull.*, 1970, **18**, 2146 (*oxide*)
Jaffari, G.A. *et al*, *J.C.S.(C)*, 1971, 4003 (*synth, uv, ir*)
Olah, G. *et al*, *J.A.C.S.*, 1972, **94**, 7438 (*oxide*)
Hyatt, J.A., *Tet. Lett.*, 1977, 141.
Alper, H. *et al*, *J. Organomet. Chem.*, 1978, **144**, C18.

1,3-Dichloroazulene, 9CI D-0-03243

[14658-94-7]



$C_{10}H_6Cl_2$ M 197.0
Mp 86-86.5°.

Nefedov, V.A., *Zh. Obshch. Khim.*, 1969, **39**, 665; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1969, **39**, 630 (*synth*)

1,5-Dichloroazulene, 9CI D-0-03244

[81971-07-5]

$C_{10}H_6Cl_2$ M 197.0
Dark blue plates. Mp 93° (89°).

Dehmlow, E.V. *et al*, *Angew. Chem., Int. Ed.*, 1982, **21**, 444 (*synth, uv, pmr*)
Dehmlow, E.V. *et al*, *Chem. Ber.*, 1985, **118**, 3805 (*synth, uv, pmr*)
Dehmlow, E.V. *et al*, *Chem. Comm.*, 1986, 1435 (*cmr*)

1,7-Dichloroazulene, 9CI D-0-03245

[99412-16-5]

$C_{10}H_6Cl_2$ M 197.0
Green needles.

Dehmlow, E.V. *et al*, *Chem. Ber.*, 1985, **118**, 3805 (*synth, uv, pmr*)

2,4-Dichloroazulene, 9CI D-0-03246

[99412-13-2]

$C_{10}H_6Cl_2$ M 197.0
Violet cryst. Mp 93°.

Dehmlow, E.V. *et al*, *Chem. Ber.*, 1985, **118**, 3805 (*synth, uv, pmr*)
Dehmlow, E.V. *et al*, *Chem. Comm.*, 1986, 1435 (*cmr*)

2,6-Dichloroazulene, 9CI D-0-03247

[81971-08-6]

$C_{10}H_6Cl_2$ M 197.0
Violet needles. Mp 141°.

Dehmlow, E.V. *et al*, *Angew. Chem., Int. Ed.*, 1982, **21**, 444 (*synth, uv, pmr*)
Dehmlow, E.V. *et al*, *Chem. Ber.*, 1985, **118**, 3805 (*synth, uv, pmr*)
Dehmlow, E.V. *et al*, *Chem. Comm.*, 1986, 1435 (*cmr*)

5,6-Dichloroazulene, 9CI D-0-03248

[63370-04-7]

$C_{10}H_6Cl_2$ M 197.0
Cryst. (EtOH aq.).

Reiter, S.E. *et al*, *J.A.C.S.*, 1977, **99**, 4199 (*synth*)
Bolton, R. *et al*, *J.C.S. Perkin 2*, 1991, 431 (*pmr*)

2,3-Dichlorobenzaldehyde D-0-03249

[6334-18-5]

$C_7H_4Cl_2O$ M 175.0
Cryst. (EtOH). Mp 65-67°.

Aldrich Library of ^{13}C *and* ^1H *FT NMR Spectra*, **2**, 947B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 113D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1294B (*ir*)
Marvel, C.S. *et al*, *J.A.C.S.*, 1946, **68**, 861.
Rahman, L.K.A. *et al*, *J.C.S. Perkin 1*, 1984, 385 (*synth*)

2,4-Dichlorobenzaldehyde D-0-03250

[874-42-0]

$C_7H_4Cl_2O$ M 175.0
Anal. reagent for carboxylic acid hydrazides. Prisms (hexane). Mp 74.5°, Mp 72°.

Oxime: [56843-28-8].

$C_7H_5Cl_2NO$ M 190.0 Needles. Mp 136-137°.

▶ CU5610500.

2,4-Dinitrophenylhydrazone: Mp 224-227°.

Anil: N-(*2,4-Dichlorobenzylidene*)aniline
$C_{13}H_9Cl_2N$ M 250.1 Yellow needles (methylcyclohexane). Mp 88-89°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 953B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 116D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1297D (*ir*)
Aldrich Library of IR Spectra, 2nd Ed., 803E (*ir*)
Aldrich Library of NMR Spectra, **6**, 88C (*pmr*)
Gindraux, L., *Helv. Chim. Acta*, 1929, **12**, 933.
Lock, G. *et al*, *Ber.*, 1937, **70**, 923.
Latour, A.A. *et al*, *Anal. Chem.*, 1964, **36**, 2479 (*use*)
Bernstein, J., *J.C.S. Perkin 2*, 1972, 946 (*cryst struct, deriv*)
Bell, R.P. *et al*, *J.C.S. Perkin 2*, 1976, 1594 (*uv*)

2,5-Dichlorobenzaldehyde D-0-03251

[6361-23-5]

$C_7H_4Cl_2O$ M 175.0
Cryst. (EtOH). Mp 58°. Bp 231-233°.

Oxime:
$C_7H_5Cl_2NO$ M 190.0 Mp 128°.

Di-Me acetal:
$C_9H_{10}Cl_2O_2$ M 221.0 d^{18} 1.274. Mp 15°. Bp 257-258°.

de Crauw, T., *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1931, **50**, 773.
Sindelar, K. *et al*, *Coll. Czech. Chem. Comm.*, 1982, **47**, 3077 (*synth*)

2,6-Dichlorobenzaldehyde D-0-03252

[83-38-5]

$C_7H_4Cl_2O$ M 175.0
Needles (petrol). Mp 71°.

Oxime: [25185-95-9].
$C_7H_5Cl_2NO$ M 190.0 Mp 149-150°.

4-Nitrophenylhydrazone: Mp 154°.

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 113C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1294A (*ir*)
Aldrich Library of IR Spectra, 2nd Ed., 802A (*ir*)
Aldrich Library of NMR Spectra, **6**, 86B (*pmr*)
Aldrich Library of NMR Spectra, 2nd edn., **2**, 112A (*nmr*)
Gindraux, L., *Helv. Chim. Acta*, 1929, **12**, 933.
Schaeffer, T., *Can. J. Chem.*, 1969, **47**, 3707.
Buchwald, P. *et al*, *Rev. Roum. Chim.*, 1974, **19**, 1221.

3,4-Dichlorobenzaldehyde D-0-03253

[6287-38-3]

$C_7H_4Cl_2O$ M 175.0
Mp 44°. Bp 247-248°. Steam-volatile.

Oxime: [5331-92-0].
$C_7H_5Cl_2NO$ M 190.0 Mp 118-119°.

4-Nitrophenylhydrazone: Mp 276-277°.

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 116C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1297C (*ir*)
Aldrich Library of IR Spectra, 2nd Ed., 803D (*ir*)
Aldrich Library of NMR Spectra, **6**, 88B (*pmr*)
Aldrich Library of NMR Spectra, 2nd edn., **2**, 114B (*nmr*)
Kraay, G.M., *Rec. Trav. Chim.* (*J. R. Neth. Chem. Soc.*), 1930, **49**, 1086.
Robev, S., *CA*, 1969, **70**, 67829r.
Bell, R.P. *et al*, *J.C.S. Perkin 2*, 1976, 1594.

3,5-Dichlorobenzaldehyde D-0-03254

[10203-08-4]

$C_7H_4Cl_2O$ M 175.0
Needles or leaflets (EtOH aq. or petrol). Mp 66°. Bp_{748} 235-240°. Steam-volatile.

Oxime:
$C_7H_5Cl_2NO$ M 190.0 Cryst. (petrol). Mp 112°.

Phenylhydrazone: Needles. Mp 106.5°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 963A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **2**, 124C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 1303A (*ir*)
Aldrich Library of IR Spectra, 2nd Ed., 806H (*ir*)
Aldrich Library of NMR Spectra, **6**, 95A (*pmr*)
Asinger, F. *et al*, *Monatsh. Chem.*, 1933, **62**, 344.
Lock, G., *Ber.*, 1939, **72**, 861.

1,2-Dichlorobenzene, 9CI D-0-03255

o-*Dichlorobenzene*, *8CI*

[95-50-1]

$C_6H_4Cl_2$ M 147.0
Liq. d_4^{20} 1.306. Mp −17°. Bp 180.5°.

▶ Irritant. Fl. p. 66°, autoignition temp. 179/180°. Can react violently with Al. Eye, skin and mucous membrane irritant. Vesicant if skin contact is prolonged. Prolonged or repeated exposure causes dizziness, headache, fatigue and may damage liver and kidneys. LD_{50} (rat, orl) 500 mg/kg. Exp. reprod. and teratogenic effects. OES: short-term 50 ppm. CZ4500000.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 68C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 976B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 893D (*ir*)
Aldrich Library of IR Spectra, 2nd Ed., 526E (*ir*)
Aldrich Library of NMR Spectra, **4**, 42A (*pmr*)
Registry of Mass Spectral Data, Wiley-Interscience, 365 (*ms*)
Sadtler Standard C-13 NMR Spectra, 1844 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 303 (*uv*)
Silberrad, O., *J.C.S.*, 1922, **121**, 1015 (*synth*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DEP600.
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworth, London and Boston, 1990, 2024.
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, Cambridge, 1992, 413.
Chemical Hazards of the Workplace, (Eds. Proctor, N.H. *et al*), 3rd edn., VNR, 1991, 215.

1,3-Dichlorobenzene, 9CI D-0-03256

m-*Dichlorobenzene*, *8CI*

[541-73-1]

$C_6H_4Cl_2$ M 147.0
Liq. d_4^{20} 1.288. Fp −26.25°. Bp 173°, Bp_8 48.5°.

▶ Fl. p. 63°. Can react violently with Al. See also comments under £00054927. CZ4499000.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 77B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 982D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 900A (*ir*)
Aldrich Library of IR Spectra, 2nd Ed., 528H (*ir*)
Aldrich Library of NMR Spectra, **4**, 46A (*pmr*)
Registry of Mass Spectral Data, Wiley-Interscience, 365 (*ms*)
Sadtler Standard C-13 NMR Spectra, 6235 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 1671 (*uv*)
Davies, W. *et al*, *J.C.S.*, 1922, **121**, 2648 (*synth*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DEP699.
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, Cambridge, 1992, 413.

1,4-Dichlorobenzene, 9CI D-0-03257

p-*Dichlorobenzene*, *8CI*, *BSI*. *Paramoth*. *Dichloricide*. *Paracide*

[106-46-7]

$C_6H_4Cl_2$ M 147.0
Insecticidal fumigant, miticide. Leaflets (EtOH) with strong odour. Mp 54°. Bp 174°.

▶ Fl. p. 66°. Possible human carcinogen. Eye and respiratory tract irritant. Prolonged or repeated exposure may damage liver and kidneys. LD_{50} (rat, orl) 500 mg/kg. Exp. carcinogen and teratogen. OES: long-term 25 ppm; short-term 50 ppm. CZ4550000.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 85B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., **1**, 988B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, **3**, 906A (*ir*)
Aldrich Library of IR Spectra, 450B (*ir*)
Registry of Mass Spectral Data, Wiley-Interscience, 365 (*ms*)
Sadtler Standard C-13 NMR Spectra, 37 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 55 (*uv*)
Silberrad, O., *J.C.S.*, 1922, **121**, 1015 (*synth*)
Burnell, E.E. *et al*, *Can. J. Chem.*, 1974, **52**, 151 (*pmr*)
Pesticide Manual, 6th edn., 1979, 169.
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DEP800.
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, Cambridge, 1992, 413.
Chemical Hazards of the Workplace, (Eds. Proctor, N.H. *et al*), 3rd edn., VNR, 1991, 216.

2,5-Dichloro-1,4-benzenedicarboxaldehyde, D-0-03258

9CI

2,5-Dichloroterephthalaldehyde, 8CI

[46052-84-0]

$C_8H_4Cl_2O_2$ M 203.0

Has herbicidal props. Yellow cryst. (EtOH aq. or $PhNO_2$). Mp 157-158° (150°).

Ruggli, P. *et al*, *Helv. Chim. Acta*, 1944, **27**, 274 (*synth*)

Naylor, J.R., *J.C.S.*, 1952, 4085 (*synth*)

U.S. Pat., 3 146 086, (1964); *CA*, **61**, 12561f (*synth*)

4,6-Dichloro-1,3-benzenedicarboxaldehyde, D-0-03259

9CI

4,6-Dichloroisophthalaldehyde, 8CI

$C_8H_4Cl_2O_2$ M 203.0

Needles (2-propanol). Mp 163-164°.

Katritzky, A.R. *et al*, *J.O.C.*, 1987, **52**, 2726 (*synth, pmr*)

2,3-Dichloro-1,4-benzenedicarboxylic acid D-0-03260

2,3-Dichloroterephthalic acid

$C_8H_4Cl_2O_4$ M 235.0

Ballester, M. *et al*, *CA*, 1963, **59**, 7082b (*synth, uv*)

2,4-Dichloro-1,3-benzenedicarboxylic acid, D-0-03261

9CI

2,4-Dichloroisophthalic acid

[50903-03-2]

$C_8H_4Cl_2O_4$ M 235.0

Mp 259°.

Weissenfels, M. *et al*, *Z. Chem.*, 1977, **17**, 56 (*synth, nmr*)

2,5-Dichloro-1,3-benzenedicarboxylic acid, D-0-03262

9CI

2,5-Dichloroisophthalic acid

[60047-46-3]

$C_8H_4Cl_2O_4$ M 235.0

Mp 255-262°.

Di-Me ester: [60047-45-2].
$C_{10}H_8Cl_2O_4$ M 263.0 Mp 108-109°.

Dichloride: [60047-44-1].
$C_8H_2Cl_4O_2$ M 271.9 Mp 38-39°.

Rondestvedt, C.S. Jr., *J.O.C.*, 1976, **41**, 3580 (*synth*)

2,5-Dichloro-1,4-benzenedicarboxylic acid D-0-03263

2,5-Dichloroterephthalic acid

[13799-90-1]

$C_8H_4Cl_2O_4$ M 235.0

Polymerisation substrate. Needles (H_2O) or by subl. Mp 306° (303°).

Mono-Me ester: [78079-32-0].
$C_9H_6Cl_2O_4$ M 249.0 Mp 173°.

Di-Me ester: [3293-89-8].
$C_{10}H_8Cl_2O_4$ M 263.0 Leaflets. Mp 137-138°.

Dichloride: [13234-55-4].
$C_8H_2Cl_4O_2$ M 271.9 Prisms (petrol). Mp 81°.

Cachia, M. *et al*, *Bull. Soc. Chim. Fr.*, 1958, 1418.

Neel, J. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 3377 (*synth*)

Otto, J. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1967, **41**, 261 (*synth*)

Japan. Pat., 74 107 397, (1974); *CA*, **84**, 123286q (*synth*)

2,6-Dichloro-1,4-benzenedicarboxylic acid D-0-03264

2,6-Dichloroterephthalic acid

$C_8H_4Cl_2O_4$ M 235.0

Ger. Pat., 2 060 604, (1971); *CA*, **75**, 89291q.

3,4-Dichloro-1,2-benzenedicarboxylic acid, D-0-03265

9CI

3,4-Dichlorophthalic acid, 8CI

$C_8H_4Cl_2O_4$ M 235.0

Plates (H_2O). Mp 195° (rapid heat). Forms anhydride at Mp.

Anhydride: [56962-07-3]. *4,5-Dichloro-1,3-isobenzofurandione*
$C_8H_2Cl_2O_3$ M 217.0 Plates. Mp 120-121°. Bp 329°.

Villiger, V., *Ber.*, 1909, **42**, 3541.

Zweig, A. *et al*, *J.O.C.*, 1978, **43**, 3690 (*pmr*)

3,5-Dichloro-1,2-benzenedicarboxylic acid D-0-03266

3,5-Dichlorophthalic acid

[25641-98-9]

$C_8H_4Cl_2O_4$ M 235.0

Needles. Mp 164°. Sublimes on heating to form the anhydride.

Di-Et ester:
$C_{12}H_{12}Cl_2O_4$ M 291.1 Bp 312-313°.

Anhydride: [51971-64-3]. *4,6-Dichloro-1,3-isobenzofurandione*
$C_8H_2Cl_2O_3$ M 217.0 Needles (petrol). Mp 89-90°.

Imide: 3,5-Dichlorophthalimide
$C_8H_3Cl_2NO_2$ M 216.0 Yellow needles (EtOH). Mp 208°.

Crossley, W.A. *et al*, *J.C.S.*, 1902, **81**, 1533.

Ponomarenko, A.A. *et al*, *J. Gen. Chem. USSR* (*Engl. Transl.*), 1950, **20**, 1911.

Verbicky, J.W. *et al*, *J.O.C.*, 1983, **48**, 2465 (*synth, pmr, cmr, deriv*)

3,6-Dichloro-1,2-benzenedicarboxylic acid D-0-03267

3,6-Dichlorophthalic acid

[16110-99-9]

$C_8H_4Cl_2O_4$ M 235.0

Plates (H_2O). pK_{a1} 1.4; pK_{a2} 3.40 (30°). Forms anhydride on heating to 100°.

Mono-Et ester:
$C_{10}H_8Cl_2O_4$ M 263.0 Mp 130-131°.

Di-Et ester:
$C_{12}H_{12}Cl_2O_4$ M 291.1 Mp 60°.

Anhydride: [4466-59-5].
$C_8H_2Cl_2O_3$ M 217.0 Mp 194.5°. Bp 339°.

Imide: 3,6-Dichlorophthalimide
$C_8H_3Cl_2NO_2$ M 216.0 Needles (H_2O). Mp 242°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 1328B (*nmr*)

Villiger, V., *Ber.*, 1902, **42**, 3539.

Palarkan, N. *et al*, *Indian J. Chem.*, 1974, **12**, 197.

Zweig, A. *et al*, *J.O.C.*, 1978, **43**, 3690 (*pmr*)

Greco, M.N. *et al*, *J.O.C.*, 1992, **57**, 5532 (*synth*)

4,5-Dichloro-1,2-benzenedicarboxylic acid D-0-03268

4,5-Dichlorophthalic acid

[56962-08-4]

$C_8H_4Cl_2O_4$ M 235.0

Needles (H_2O). Mp *ca.* 200° (forms anhydride).

Mono-Et ester:
$C_{10}H_8Cl_2O_4$ M 263.0 Needles ($CHCl_3$). Mp 133-134°.

Anhydride: [942-06-3].
$C_8H_2Cl_2O_3$ M 217.0 Mp 185-187°. Bp 313°.

[15997-89-4]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, **2**, 1154C, 1328C (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., **2**, 235A (*ir*)

Villiger, V., *Ber.*, 1909, **42**, 3546.

Ayling, E.E. *et al*, *J.C.S.*, 1929, 253.

Zweig, A. *et al*, *J.O.C.*, 1978, **43**, 3690 (*synth, pmr*)

Verbicky, J.W. *et al*, *J.O.C.*, 1983, **48**, 2465 (*derivs, synth*)

Caswell, L.R. *et al*, *Synthesis*, 1992, 823 (*anhydride, synth, ir, pmr*)

4,5-Dichloro-1,3-benzenedicarboxylic acid, D-0-03269

9CI

4,5-Dichloroisophthalic acid

[6660-66-8]

$C_8H_4Cl_2O_4$ M 235.0

Mp 305-306°.

Di-Me ester: [60047-49-6].
$C_{10}H_8Cl_2O_4$ M 263.0 Mp 79-80°.

Dichloride: [60047-48-5].
$C_8H_2Cl_4O_2$ M 271.9 Mp 37-38°.

Rondestvedt, C.S. Jr., *J.O.C.*, 1976, **41**, 3580 (*synth*)

4,6-Dichloro-1,3-benzenedicarboxylic acid, D-0-03270

9CI

4,6-Dichloroisophthalic acid

[6660-65-7]

$C_8H_4Cl_2O_4$ M 235.0

Mp 280°, Mp 353-356°.

Di-Me ester: [60047-50-9].
$C_{10}H_8Cl_2O_4$ M 263.0 Mp 98-101°.

Dichloride: [2855-01-8].
$C_8H_2Cl_4O_2$ M 271.9 Mp 76-77°.

Anilide:
$C_{14}H_9Cl_2NO_3$ M 310.1 Mp 205°.

Pollack, J. *et al*, *Monatsh. Chem.*, 1922, **43**, 209 (*synth*)