

# 3

Third edition

## Ashford's Dictionary of Industrial Chemicals



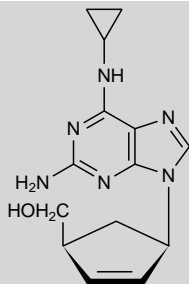
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1

Dictionary

# abacavir

Ziagen (GlaxoSmithKline); [136470-78-5]; [188062-50-2] (2:1 sulfate salt)



$C_{14}H_{18}N_6O_1$  (286.33). Available commercially as the 2:1 sulfate salt.

## Uses

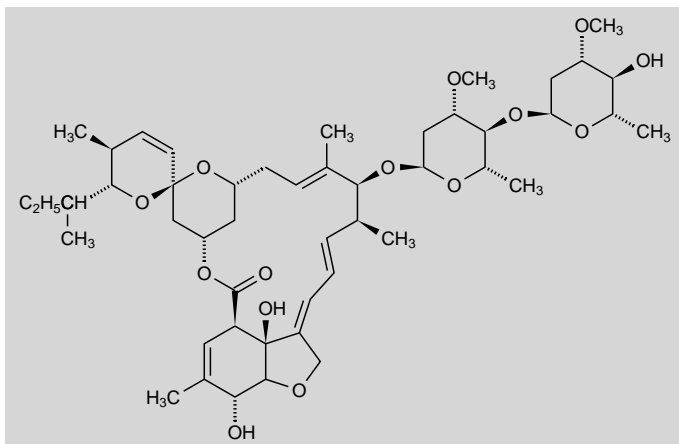
HIV therapy drug

## Production

- 2-amino-4,6-dichloropyrimidine + (1*R*,4*S*)-2-azabicyclo[2.2.1]hept-5-en-3-one + trimethyl orthoformate + cyclopropylamine (N-protection/nitrosation/nitro reduction/ N-protection/amide hydrolysis/carboxyl reduction/ amine formation/cyclisation/amine formation/ deprotection)
- (1*RS*,4*SR*)-2-azabicyclo[2.2.1]hept-5-en-3-one + 2-amino-4,6-dichloropyrimidine + trimethyl orthoformate + cyclopropylamine (amide hydrolysis/ester formation/N-acetylation/enantiomer separation/ carboxyl reduction/N-protection/nitrosation/amine formation/nitro reduction/cyclisation/amine formation/ deprotection)

# abamectin

avermectin B<sub>1</sub>; [71751-41-2]



C<sub>48</sub>H<sub>72</sub>O<sub>14</sub> (873.08). Impure mixture comprising mainly avermectin B<sub>1a</sub>.

## Uses

insecticide/acaricide/nematicide

## Production

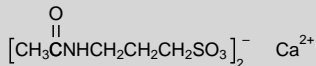
- microbial fermentation medium + *Streptomyces avermitilis* actinomycete (fermentation/extraction)

## Derivatives

emamectin benzoate  
epinomectin  
ivermectin

# acamprosate calcium

3-acetamidopropylsulfonic acid, calcium salt; calcium 3-acetamidopropylsulfonate; [77337-73-6]



$\text{C}_{10}\text{H}_{20}\text{Ca}_1\text{N}_2\text{O}_8\text{S}_2$  (400.48).

## Uses

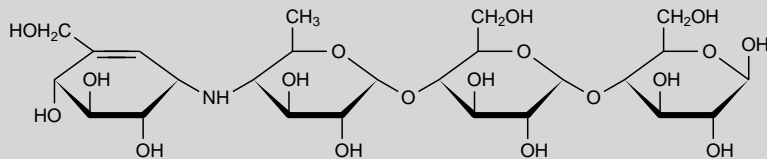
alcohol dependence therapy drug

## Production

- 3-aminopropanol + acetic anhydride + sodium hydro-sulfide (N-acetylation/alcohol chlorination/thiol formation/sulfide oxidation/calcium salt formation)

# acarbose

[56180-94-0]



$C_{25}H_{43}N_1O_{18}$  (645.60).

## Uses

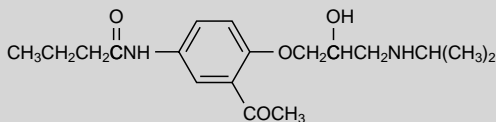
invertase inhibitor drug (diabetes treatment)

## Production

- microbial fermentation medium + *Actinoplanes* spp. (fermentation/extraction/chromatographic purification)

# acebutolol

[37517-30-9]



C<sub>18</sub>H<sub>28</sub>N<sub>2</sub>O<sub>4</sub> (336.43). Available commercially as the hydrochloride salt.

## Uses

β-receptor blocker drug

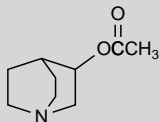
## Production

- *N*-butyryl-*p*-aminophenol + acetic anhydride + epichlorohydrin + isopropylamine (O-acetylation/Fries rearrangement/epoxidation/amine formation)



# aceclidine

3-quinuclidinyl acetate; [827-61-2]; 212-574-1 (EC)



$C_9H_{15}N_1O_2$  (169.22).

## Uses

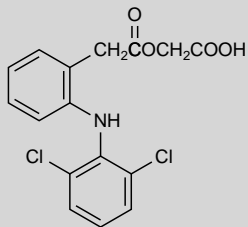
antihypertensive drug

## Production

- 3-quinuclidinol + acetic anhydride (ester formation)

# aceclofenac

2-[(2,6-dichlorophenyl)amino]phenylacetoacetic acid; [89796-99-6]



$C_{16}H_{13}Cl_2N_1O_4$  (354.18).

## Uses

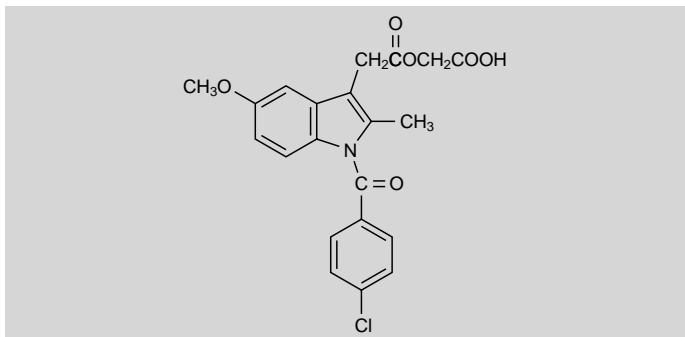
antiinflammatory drug

## Production

- diclofenac + glycollic acid (acid chloride formation/ ester formation)

# acemetacin

[53164-05-9]



$C_{21}H_{18}Cl_1N_1O_6$  (415.82).

## Uses

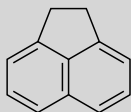
antiinflammatory drug

## Production

- indometacin + glycollic acid (acid chloride formation/ ester formation)

# acenaphthene

[83-32-9]



$C_{12}H_{10}$  (154.21). Crystalline solid. MP: 92–95°C. BP: 279°C. d: 1.20 kg/l (20°C). Insoluble in water. Soluble in chlorinated and aromatic solvents.

## Production

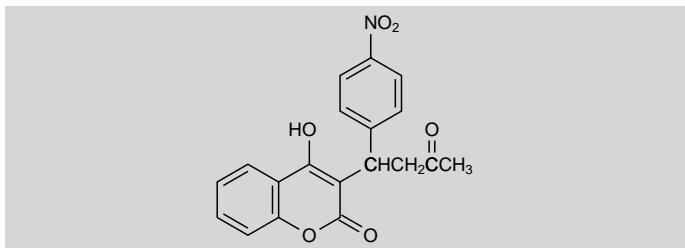
- heavy coal tar oil (fractionation; coproduced with methylnaphthalene fraction/dimethylnaphthalene fraction/naphthalene fraction)

## Derivatives

memantine  
naphthalene-1,4,5,8-tetracarboxylic acid  
naphthalic anhydride  
naphthalic anhydride-4-sulfonic acid  
Sulfur Brown 52

# acenocoumarol

nicoumalone; [152-72-7]



$C_{19}H_{15}N_1O_6$  (353.33).

## Uses

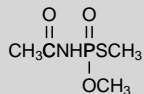
anticoagulant drug

## Production

- *p*-nitrobenzaldehyde + acetone + 4-hydroxycoumarin (aldol condensation/Michael addition)

# acephate

acetylphosphoramidothioic acid, O,S-dimethyl ester; O,S-dimethyl acetylphosphoramidothioate; [30560-19-1]



$C_4H_{10}N_1O_3P_1S_1$  (183.17).

## Uses

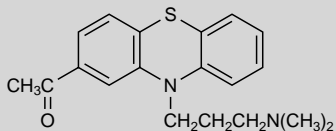
insecticide

## Production

- acetic anhydride + methamidophos (amide formation)

# acepromazine

2-acetyl-10-(3-dimethylaminopropyl)phenothiazine; [3598-37-6] (maleate); [61-00-7]



$C_{19}H_{22}N_2O_1S_1$  (326.46). Available commercially as the (1:1) maleate salt.

## Uses

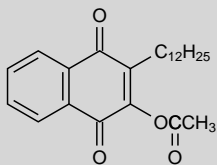
veterinary tranquilliser drug

## Production

- phenothiazine + acetyl chloride + 3-(dimethylamino)propyl chloride hydrochloride (amide formation/Friedel-Crafts acylation/amide hydrolysis/amine formation)

# acequinocyl

3-dodecyl-1,4-dihydro-1,4-dioxo-2-naphthyl acetate; [57960-19-7]



C<sub>24</sub>H<sub>32</sub>O<sub>4</sub> (384.51).

## Uses

acaricide/miticide

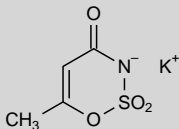
## Production

- β-naphthol + 1-dodecene + acetic acid (oxidation/  
Friedel-Crafts alkylation/O-acetylation)



# acesulfame-K

acesulfame-potassium; E950 (EC); [55589-62-3]



$C_4H_4K_1N_1O_4S_1$  (201.24). White crystals. MP: 250°C. Soluble in water.

## Uses

artificial sweetener

## Production

- diketene + sulfamic acid + potassium carbonate (cyclisation/salt formation)

# acetaldehyde

ethanal; [75-07-0]

CH<sub>3</sub>CHO

C<sub>2</sub>H<sub>4</sub>O<sub>1</sub> (44.05). Colourless gas or liquid with a pungent odour. BP: 20°C. MP: -124°C. d: 0.79 kg/l (15°C). Miscible with water, oxygenated and aromatic solvents.

## Production

- ethylene + air (Wacker-Celanese two-step oxidation process)
- oxygenates, Fischer-Tropsch, mixed (fractionation; coproduced with methanol/ethanol/acetone/acetic acid/isopropanol/*n*-propanol/methyl ethyl ketone/*n*-butanol)
- ethanol + air (catalytic oxidation)
- ethylene + oxygen (Wacker-Celanese single-step oxidation process)
- vinyl acetate (ester hydrolysis/isomerisation)

## Derivatives

acetaldehyde oxime  
acetic acid  
acetic anhydride  
6-acetoxy-2,4-dimethyl-1,3-dioxane  
Acid Yellow 5  
D-alanine  
DL-alanine  
L-alanine  
benzophenonetetracarboxylate dianhydride  
bethoxazin  
1,3-butanediol  
4-*t*-butyldihydrocinnamaldehyde  
1-butyn-3-ol  
cefprozil

# acetaldehyde

ethanal; [75-07-0]

## Derivatives (Continued)

1-chloroethyl cyclohexyl carbonate  
1-chloroethyl ethyl carbonate  
7-chloroquinoline  
cinnamaldehyde  
crotonaldehyde  
crotonylidene urea  
diethyl ethylmalonate  
diisopropyl ketone  
eletriptan  
ethyl acetate  
2-ethylbutyraldehyde  
2,2'-ethylidene bis(4,6-di-*t*-butylphenol)  
etodolac  
furametpyr  
glyoxal  
2,5-hexynediol  
indaziflam  
*p*-isobutylstyrene  
isocyclemone  
DL-lactic acid  
lofexidine  
metaldehyde  
methohexital  
methyl *n*-butyl ketone  
3,4-methylenedioxy-*N*-ethylaniline  
2-methylimidazole  
methyl isopropyl ketone

# acetaldehyde

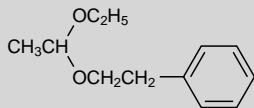
ethanal; [75-07-0]

## Derivatives (Continued)

methyl propyl ketone  
netilmicin  
paraldehyde  
pentaerythritol  
 $\alpha$ -picoline  
 $\beta$ -picoline  
 $\gamma$ -picoline  
pyridine  
pyrvinium pamoate  
quinaldine  
(*Z,E*)-tetradeca-9,12-dienyl acetate  
verbutin  
vinyl acetate  
*N*-vinylformamide

# acetaldehyde ethyl phenethyl diacetal

Verdilyn (Givaudan); [2556-10-7]; 219-868-9 (EC)



C<sub>12</sub>H<sub>18</sub>O<sub>2</sub> (194.27).

## Uses

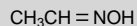
fragrance ingredient

## Production

- ethyl vinyl ether + phenethyl alcohol (alcohol addition)

# acetaldehyde oxime

acetaldoxime; [107-29-9]



$\text{C}_2\text{H}_5\text{N}_1\text{O}_1$  (59.07). Solid. MP: 44–46°C. BP: 115°C. Soluble in warm water, oxygenated and chlorinated solvents. Commercial grades contain 90–95% of the *anti*-isomer.

## Production

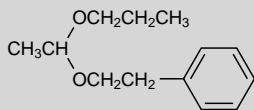
- acetaldehyde + hydroxylamine sulfate (oxime formation)

## Derivatives

methomyl  
thiodicarb

# acetaldehyde *n*-propyl phenethyl diacetal

Acetal R (Givaudan); [7493-57-4]; 231-327-9 (EC)



$C_{13}H_{20}O_2$  (208.30). Clear liquid with a hyacinth-like smell.

## Uses

fragrance ingredient

## Production

- acetylene + *n*-propanol + phenethyl alcohol (ethynylation/alcohol addition)

# acetamide

[60-35-5]



$\text{C}_2\text{H}_5\text{N}_1\text{O}_1$  (59.07). White crystals. MP: 82°C. BP: 221°C. d: 1.00 kg/l (85°C). Soluble in water and alcohol.

## Uses

solubiliser; solvent

## Production

- ammonium acetate (dehydration)

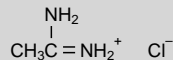
## Derivatives

*N*-acetylpiperazine



# acetamidine hydrochloride

[124-42-5]



$\text{C}_2\text{H}_7\text{Cl}_1\text{N}_2$  (94.54). Prepared *in situ*. Not a commercially-traded product. Dissociates into acetic acid and ammonia on warming. Soluble in water and alcohol.

## Production

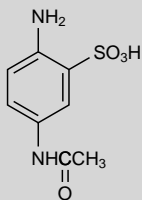
- acetonitrile + ammonia + hydrochloric acid (nitrile addition/salt formation)

## Derivatives

4-amino-5-aminomethyl-2-methylpyrimidine  
4-amino-5-ethoxymethyl-2-methylpyrimidine  
moxonidine

# 5-acetamido-2-aminobenzenesulfonic acid

4-aminoacetanilide-3-sulfonic acid; [96-78-6]; 202-534-1 (EC)



$C_8H_{10}N_2O_4S_1$  (230.24).

## Uses

dyestuffs intermediate

## Production

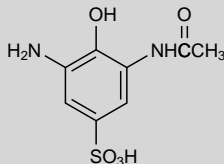
- 2,5-diaminobenzenesulfonic acid + acetic anhydride (N-acetylation)

## Derivatives

Reactive Orange 14

## 6-acetamido-2-aminophenol-4-sulfonic acid

3-(acetamino)-5-amino-4-hydroxybenzenesulfonic acid; 3-acetamido-2-hydroxyaniline-5-sulfonic acid; [40306-75-0]; 254-879-2 (EC)



$C_8H_{10}N_2O_5S_1$  (246.24). Pale pink powder.

### Uses

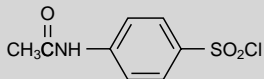
dyestuffs intermediate

### Production

- acetic anhydride + 2-aminophenol-4-sulfonic acid (N-acetylation/ring nitration/nitro reduction)

# 4-acetamidobenzenesulfonyl chloride

*N*-acetylsulfanilyl chloride; [121-60-8]; 204-485-1 (EC)



C<sub>8</sub>H<sub>8</sub>Cl<sub>1</sub>N<sub>1</sub>O<sub>3</sub>S<sub>1</sub> (233.67). Light brown powder. MP: 146–148°C with decomposition. Hydrolysed by water. Soluble in chlorinated and aromatic solvents.

## Production

- acetanilide + chlorosulfonic acid (chlorosulfonation)

## Derivatives

4-acetylsulfanilamide  
Acid Black 234  
amprenavir  
4,4'-diaminobenzenesulfanilide  
fosamprenavir  
sulfabenzamide  
sulfadicramide  
sulfadimethoxine  
sulfadimidine  
sulfadoxine  
sulfafurazole  
sulfaguanidine  
sulfaisodimidine  
sulfamerazine  
sulfamethizole  
sulfamethoxazole  
sulfametomidine  
sulfamonomethoxine  
sulfamoxole  
sulfaperin  
sulfaphenazole  
sulfapyridine  
sulfaquinoxaline

# 4-acetamidobenzenesulfonyl chloride

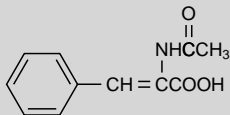
*N*-acetylsulfanilyl chloride; [121-60-8]; 204-485-1 (EC)

Derivatives (Continued)

sulfathiazole

## 2-acetamidocinnamic acid

ACA; [5469-45-4]



$C_{11}H_{11}N_1O_3$  (205.21). Solid. Available as the dihydrate.  
MP: 185–186°C. Soluble in water.

### Production

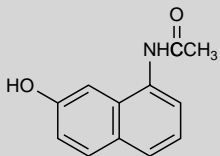
- acetic anhydride + glycine + benzaldehyde (N-acetylation/condensation)

### Derivatives

L-phenylalanine

# 1-acetamido-7-naphthol

1-acetamido-7-hydroxynaphthalene; 8-acetamido-2-hydroxynaphthalene; [6470-18-4]; 229-293-5 (EC)



$C_{12}H_{11}N_1O_2$  (201.22).

## Production

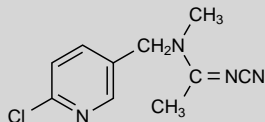
- 1,7-Cleve's acid + acetic anhydride (N-acetylation/alkali fusion)

## Derivatives

Acid Black 60  
Acid Blue 171  
Acid Brown 227  
Acid Brown 436  
Mordant Black 38

# acetamiprid

*N*-[6-chloro-3-pyridylmethyl]-*N'*-cyano-*N*-methylacetamidine; [135410-20-7]



$C_{10}H_{11}Cl_1N_4$  (222.67).

## Uses

insecticide

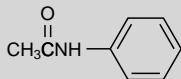
## Production

- acetonitrile + cyanamide + 6,α-dichloro-β-picoline (amidine formation/*N*-methylation/amine formation)



# acetanilide

*N*-phenylacetamide; [103-84-4]; 203-150-7 (EC)



$C_8H_9N_1O_1$  (135.16). White, crystalline solid. MP: 113–115°C. BP: 304–307°C. d: 1.21 kg/l (4°C). Soluble in hot water and oxygenated solvents.

## Production

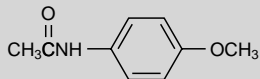
- acetic acid + aniline (N-acetylation)

## Derivatives

4-acetamidobenzenesulfonyl chloride  
*p*-bromoaniline  
Disperse Red 136  
*p*-nitroacetanilide  
*o*-nitroaniline  
*p*-nitroaniline  
2,4,6-trichlorophenylhydrazine

## acet-*p*-anisidide

*N*-acetyl-*p*-aminoanisole; *p*-acetamidoanisole; 4-methoxyacetanilide; [51-66-1]



$C_9H_{11}N_1O_2$  (165.19). Solid. MP: 131°C. Slightly soluble in water. Soluble in oxygenated solvents.

### Production

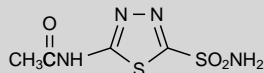
- acetic anhydride + *p*-anisidine (amide formation)

### Derivatives

4-amino-3-nitroanisole

# acetazolamide

[59-66-5]



C<sub>4</sub>H<sub>6</sub>N<sub>4</sub>O<sub>3</sub>S<sub>2</sub> (222.25).

## Uses

carbonic anhydrase inhibitor drug (diuretic/antiepileptic/  
glaucoma treatment)

## Production

- hydrazine + ammonium thiocyanate + acetic anhydride + ammonia (thiocyanate addition/cyclisation/N-acetylation/oxidation/sulfonamide formation)

# acetic acid

E260 (EC); [64-19-7]

CH<sub>3</sub>COOH

C<sub>2</sub>H<sub>4</sub>O<sub>2</sub> (60.05). Colourless liquid or solid with a characteristic, sharp odour. MP: 16°C. BP: 117–118°C. d: 1.05 kg/l (20°C). Miscible with water and oxygenated solvents. Flash point: 57°C (OC). Also available as a 60% solution in water and in a ~5% solution as vinegar.

## Uses

process solvent (hydrogenation, nitration, diazotisation, terephthalic acid production); dyeing auxiliary; etchant (semiconductor manufacture); laundry sour; Mitsubishi 1,4-butanediol process reagent; Showa Denka allyl alcohol process reagent; acidulant (pickles, sauces, ketchup); aluminium brightening agent

## Production

- acetaldehyde (liquid-phase air oxidation process)
- acetaldehyde + oxygen (liquid-phase oxidation process; coproduced with acetic anhydride)
- methanol + carbon monoxide (methanol carbonylation processes)
- acetic anhydride + salicylic acid (O-acetylation; byproduct of acetylsalicylic acid production)
- acetic anhydride + *p*-aminophenol (N-acetylation; byproduct of paracetamol production)
- poly(vinyl acetate) (ester hydrolysis; byproduct of poly(vinyl alcohol) production)
- acetic anhydride + bleached wood pulp/cotton linters (ester formation/partial hydrolysis; byproduct of cellulose acetate production)
- methyl acetate/methanol + carbon monoxide (methyl acetate carbonylation processes; coproduced with acetic anhydride)
- ethylene + vinyl acetate (polymerisation/ester hydrolysis; byproduct of ethylene-vinyl alcohol copolymers production)
- oxygenates, Fischer-Tropsch, mixed (fractionation; coproduced with methanol/acetaldehyde/ethanol/acetone/isopropanol/*n*-propanol/methyl ethyl ketone/*n*-butanol)

# acetic acid

E260 (EC); [64-19-7]

## Production (Continued)

- poly(vinyl acetate) (methanol transesterification/ester hydrolysis; byproduct of poly(vinyl alcohol) production)
- naphtha, heavy (liquid-phase oxidation process; coproduced with formic acid/acetone/methyl ethyl ketone/propionic acid)
- vinyl acetate (ester hydrolysis/isomerisation; byproduct of acetaldehyde production)

## Derivatives

acequinocyl  
acetanilide  
acetic anhydride  
*N*-(2-acetoxyethyl)-*N*-(2-cyanoethyl)aniline  
acetyl chloride  
acetylcholine chloride  
acrinathrin  
allyl acetate  
aluminium acetate  
aluminium acetate, basic  
ammonium acetate  
amyl acetate  
anisyl acetate  
antimony triacetate  
benzoyl chloride  
benzyl acetate

# acetic acid

E260 (EC); [64-19-7]

## Derivatives (Continued)

bornyl acetate  
bromoacetic acid  
bromoacetyl bromide  
*n*-butyl acetate  
*s*-butyl acetate  
calcium acetate  
calcium magnesium acetate  
chloroacetic acid  
cinnamyl acetate  
citronellyl acetate  
cobalt acetate  
cocoamine acetate  
copper acetate  
*trans*-dec-5-enyl acetate  
diacetin  
diacetyl fatty acid monoglyceride tartrate  
dibutyltin diacetate  
dicyclopentenyl acetate  
diethyl acetamidomalonate  
diethylene glycol monobutyl ether acetate  
diethylene glycol monoethyl ether acetate  
dimethylacetamide  
Disperse Red 74  
Disperse Red 82  
Disperse Red 135  
Disperse Red 151  
Disperse Red 167

# acetic acid

E260 (EC); [64-19-7]

## Derivatives (Continued)

Disperse Red 167:1  
Disperse Red 202  
Disperse Violet 33  
dodeca-7,9-dienyl acetate  
dodeca-8,10-dienyl acetate  
(Z)-dodec-7-enyl acetate  
(Z)-dodec-8-enyl acetate  
(Z)-dodec-9-enyl acetate  
dodemorph acetate  
dodine  
eprinomectin  
ethyl acetate  
ethylene glycol diacetate  
ethylene glycol monobutyl ether acetate  
ethylene glycol monoethyl ether acetate  
ethylene glycol monomethyl ether acetate  
2-ethylhexyl acetate  
famciclovir  
fatty acid glycerides, acetylated  
3-formylcrotonyl acetate  
geranyl acetate  
gossypure  
guazatine acetate  
(Z)-hexadec-11-enyl acetate  
(Z)-hexadec-13-en-11-ynyl acetate  
2-hexenyl acetate  
3-hexenyl acetate

# acetic acid

E260 (EC); [64-19-7]

## Derivatives (Continued)

hexyl acetate  
*n*-hexyl acetate  
isoamyl acetate  
isobornyl acetate  
isobutyl acetate  
isoheptyl acetate  
L-isoleucine  
isononyl acetate  
isopropyl acetate  
ketene  
lanolin, acetylated  
lanolin alcohol, acetylated  
lavandulyl acetate  
lead acetate  
linalyl acetate  
lithium acetate  
L-lysine  
magnesium acetate  
mercuric acetate  
3-methoxybutyl acetate  
*N*-methylacetamide  
2-methylbenzothiazole  
2-methylcyclohexyl acetate  
methyl triacetoxysilane  
nickel acetate  
octadeca-2,13-dienyl acetate  
peracetic acid



# acetic acid

E260 (EC); [64-19-7]

## Derivatives (Continued)

phenethyl acetate  
phenyl acetate  
1-phenylethyl acetate  
3-phenylpropyl acetate  
pinacolone  
potassium acetate  
*n*-propyl acetate  
propylene glycol monoethyl ether acetate  
propylene glycol monomethyl ether acetate  
roxatidine acetate  
sodium acetate  
stearylamine acetate  
tallowamine acetate  
tebufloquin  
(*E,Z*)-tetradeca-4,10-dienyl acetate  
(*Z,E*)-tetradeca-9,11-dienyl acetate  
(*Z,E*)-tetradeca-9,12-dienyl acetate  
(*Z*)-tetradec-9-enyl acetate  
tetradec-11-enyl acetate  
triacetin  
tri-*n*-butyl acetylcitrate  
tributyltin acetate  
trichloroacetic acid  
tridec-4-en-1-yl acetate  
triethyl acetylcitrate  
triethylene glycol diacetate  
trifluoroacetic acid

# acetic acid

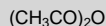
E260 (EC); [64-19-7]

## Derivatives (Continued)

vinyl acetate  
vinyltriacetoxysilane  
zinc acetate  
zirconium acetate

# acetic anhydride

[108-24-7]



$\text{C}_4\text{H}_6\text{O}_3$  (102.09). Colourless liquid with an acetic odour. BP: 139°C. MP: -74°C. d: 1.08 kg/l (20°C). Slowly hydrolysed by water and alcohols to acetic acid and esters. Soluble in oxygenated and chlorinated solvents.

## Uses

reagent (acetylation, condensation, dehydration); semiconductor processing reagent; acetic acid chlorination catalyst; acetyl chloride raw material (*in situ* production); aluminium electrolytic polishing agent

## Production

- acetic acid + ketene (addition)
- acetaldehyde + oxygen (liquid-phase oxidation process; coproduced with acetic acid)
- methanol + carbon monoxide/methyl acetate (methyl acetate carbonylation processes; coproduced with acetic acid)
- methyl acetate + carbon monoxide (carbonylation)

## Derivatives

acamprosate calcium  
acebutolol  
aceclidine  
acephate  
5-acetamido-2-aminobenzenesulfonic acid  
6-acetamido-2-aminophenol-4-sulfonic acid  
2-acetamidocinnamic acid  
1-acetamido-7-naphthol  
acet-*p*-anisidide  
acetazolamide  
acetohydrazide  
acetohydroxamic acid  
6-acetoxy-2,4-dimethyl-1,3-dioxane  
*N*-acetyl-L-cysteine  
*N*-acetylethanolamine  
acetyl-gamma acid

# acetic anhydride

[108-24-7]

## Derivatives (Continued)

*N*-acetylglucosamine  
*N*-acetyl-H acid  
1-acetyl-4-(4'-hydroxyphenyl)piperazine  
acetyl-J acid  
2-acetyl-6-methoxynaphthalene  
*N*-acetylsalicylamide  
acetylsalicylic acid  
*N*-acetylthiazolidine-4-carboxylic acid  
2-acetylthiophene  
*N*-acetyl-*o*-toluidine  
4-acetyl-1,1,6-trimethylethanoctahydronaphthalene  
Acid Red 82  
amidotrizoic acid  
*m*-aminoacetanilide  
*p*-aminoacetanilide  
2-amino-5-nitrophenol  
L- $\alpha$ -aminovaleric acid  
baclofen  
Basic Yellow 24  
bisacodyl  
*N*-butylacetanilide  
2-*t*-butylcyclohexyl acetate  
4-*t*-butylcyclohexyl acetate  
cedryl acetate  
cedryl methyl ketone  
celiprolol  
cellulose acetate

# acetic anhydride

[108-24-7]

## Derivatives (Continued)

cellulose acetobutyrate  
cellulose propionate  
cellulose triacetate  
cinnamic acid  
coumarin  
cuelure  
decahydro- $\beta$ -naphthyl acetate  
3,5-diacetoxyacetophenone  
diamorphine  
difethialone  
diflufenzopyr  
dihydroterpinyl acetate  
2,6-dihydroxyacetophenone  
2,4-dihydroxyquinoline  
diltiazem  
dimethomorph  
dimethyl benzyl carbonyl acetate  
disodium 4,4'-bis(3,5-dimethyl-6-sulfobenzofuran-2-yl)-  
biphenyl  
Disperse Blue 79  
Disperse Blue 79:1  
Disperse Blue 130  
Disperse Blue 281  
Disperse Blue 291  
Disperse Blue 291:1  
Disperse Red 324  
Disperse Yellow 77

# acetic anhydride

[108-24-7]

## Derivatives (Continued)

donepezil  
eprosartan  
esmolol  
ethopabate  
2-ethoxyethyl *p*-methoxycinnamate  
2-ethylhexyl *p*-methoxycinnamate  
eugenyl acetate  
flumorph  
Food Black 1  
guaiyl acetate  
7-hydroxycoumarin  
hydroxyethylidene(diphosphonic acid)  
2-hydroxy-5-nonylacetoxyphenoxime  
iminostilbene  
iocetamic acid  
iohexol  
iotalamic acid  
*p*-isobutylacetophenone  
levodopa  
linezolid  
lorazepam  
mafenide  
mefluidide  
Meldrum's acid  
menthyl acetate  
4-methoxyacetophenone  
o-methylacetophenone

# acetic anhydride

[108-24-7]

## Derivatives (Continued)

*p*-methylacetophenone  
metipranolol  
metolazone  
midazolam  
musk ketone  
nedocromil  
*p*-nitroacetanilide  
5-nitrofurfural diacetate  
nopyl acetate  
oseltamivir  
oxazepam  
paracetamol  
pentaacetylglucose  
phenacetin  
Pigment Violet 37  
polyacetal, homopolymers  
pyrifluquinazon  
raltitrexed  
silaflofen  
Solvent Red 52  
starch acetate  
sucrose acetate isobutyrate  
sucrose octaacetate  
sulcotrione  
sulfacetamide  
Sulfur Yellow 9  
temazepam

# acetic anhydride

[108-24-7]

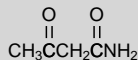
## Derivatives (Continued)

terpinyl acetate  
tetraacetylenediamine  
tetrahydrolinalyl acetate  
thioacetic acid  
 $\alpha$ -tocopheryl acetate  
triacetin  
 $\alpha$ -trichloromethylphenyl carbonyl acetate  
vetiveryl acetate  
vinyl acetate  
zaleplon  
zanamivir  
zolmitriptan



# acetoacetamide

BKB;  $\beta$ -ketobutyramide; [5977-14-0]; 227-774-4 (EC)



$\text{C}_4\text{H}_7\text{N}_1\text{O}_2$  (101.10). Available commercially as a dark yellow solution in water containing 30% active matter.

## Uses

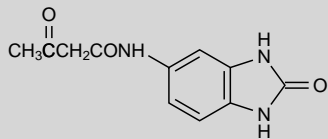
formaldehyde scavenger

## Production

- diketene + ammonia (amide formation)

# 5-acetoacetamidobenzimidazolone

[26576-46-5]



$C_{11}H_{11}N_3O_3$  (233.22).

## Production

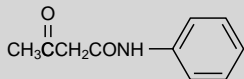
- diketene + 5-aminobenzimidazolone (amide formation)

## Derivatives

Pigment Orange 36  
Pigment Yellow 120  
Pigment Yellow 151  
Pigment Yellow 154  
Pigment Yellow 180  
Pigment Yellow 181

# acetoacetanilide

AAA; [102-01-2]; 202-996-4 (EC)



C<sub>10</sub>H<sub>11</sub>N<sub>1</sub>O<sub>2</sub> (177.20). White or pale yellow crystalline powder. MP: 85–86°C. Slightly soluble in water. Soluble in oxygenated and chlorinated solvents.

## Production

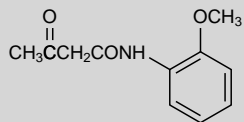
- diketene + aniline (amide formation)

## Derivatives

Acid Green 111  
Acid Yellow 44  
Acid Yellow 128  
Acid Yellow 151  
Acid Yellow 194  
carboxin  
Direct Yellow 8  
fenfuram  
Pigment Orange 15  
Pigment Orange 16  
Pigment Yellow 1  
Pigment Yellow 4  
Pigment Yellow 5  
Pigment Yellow 12  
Pigment Yellow 126  
rebamipide  
Solvent Orange 45  
Solvent Yellow 19

# acetoacet-o-anisidide

AAOA; *o*-acetoacetanisidide; [92-15-9]



C<sub>11</sub>H<sub>13</sub>N<sub>1</sub>O<sub>3</sub> (207.23). Solid. MP: 83°C.

## Production

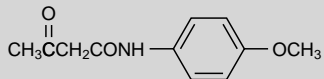
- diketene + *o*-anisidine (amide formation)

## Derivatives

Direct Yellow 27  
Pigment Yellow 17  
Pigment Yellow 65  
Pigment Yellow 73  
Pigment Yellow 74

# acetoacet-*p*-anisidide

*p*-acetoacetanisidide; [5437-98-9]; 226-615-6 (EC)



C<sub>11</sub>H<sub>13</sub>N<sub>1</sub>O<sub>3</sub> (207.23).

## Production

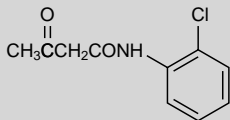
- diketene + *p*-anisidine (amide formation)

## Derivatives

Pigment Yellow 126  
Pigment Yellow 170

# acetoacet-o-chloroanilide

2'-chloroacetoacetanilide; AAOC; [93-70-9]; 202-269-1 (EC)



C<sub>10</sub>H<sub>10</sub>ClN<sub>1</sub>O<sub>2</sub> (211.64). White, crystalline powder. MP: 103°C.

## Production

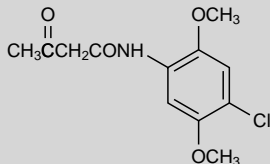
- diketene + *o*-chloroaniline (amide formation)

## Derivatives

Acid Green 73  
Acid Yellow 116  
Acid Yellow 220  
Pigment Yellow 3

# acetoacet-4-chloro-2,5-dimethoxyanilide

AADMC; acetoacet-2,5-dimethoxy-4-chloroanilide; [4433-79-8]; 224-638-6 (EC)



$C_{12}H_{14}Cl_1N_1O_4$  (271.70).

## Production

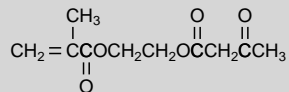
- diketene + 4-chloro-2,5-dimethoxyaniline (amide formation)

## Derivatives

Pigment Yellow 83  
Pigment Yellow 97  
Pigment Yellow 176

## 2-(acetoacetoxyethyl) methacrylate

AAEM; methacryloxyethyl acetoacetate; [21282-97-3]; 244-311-1 (EC)



$\text{C}_{10}\text{H}_{14}\text{O}_5$  (214.22).

### Uses

crosslinking comonomer (acrylic powder coatings)

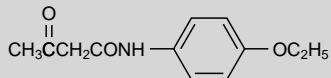
### Production

- methyl acetoacetate + 2-hydroxyethyl methacrylate (transesterification)



# acetoacet-*p*-phenetidine

AAPP; 4-ethoxyacetoacetanilide; [122-82-7]; 204-577-1 (EC)



$C_{12}H_{15}N_1O_3$  (221.25). White, crystalline powder. MP: 102°C.

## Production

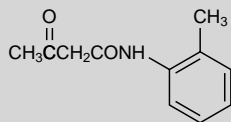
- diketene + *p*-phenetidine (amide formation)

## Derivatives

Pigment Yellow 75

# acetoacet-*o*-toluidide

AAOT; [93-68-5]; 202-267-0 (EC)



C<sub>11</sub>H<sub>13</sub>N<sub>1</sub>O<sub>2</sub> (191.23).

## Production

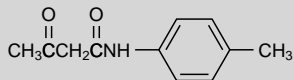
- diketene + *o*-toluidine (amide formation)

## Derivatives

- Pigment Orange 1
- Pigment Yellow 14
- Pigment Yellow 62
- Pigment Yellow 174

# acetoacet-*p*-toluidide

4'-methylacetoacetanilide; AAPT; [1503-54-4]; 216-127-1 (EC)



C<sub>11</sub>H<sub>13</sub>N<sub>1</sub>O<sub>2</sub> (191.23). White crystals. MP: 95°C. Soluble in oxygenated and aromatic solvents.

## Production

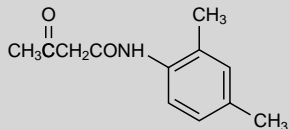
- diketene + *p*-toluidine (amide formation)

## Derivatives

Pigment Yellow 55

# acetoacet-2,4-xylylide

2'4'-dimethylacetoacetanilide; AAMX; acetoacet-*m*-xylylide; [97-36-9]; 202-576-0 (EC)



C<sub>12</sub>H<sub>15</sub>N<sub>1</sub>O<sub>2</sub> (205.25).

## Production

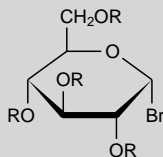
- diketene + 2,4-xylylidine (amide formation)

## Derivatives

Pigment Yellow 13  
Pigment Yellow 81  
Pigment Yellow 127  
Pigment Yellow 174  
Pigment Yellow 176

# $\alpha$ -acetobromo-D-glucose

2,3,4,6-tetra-O-acetyl- $\alpha$ -D-glucopyranosyl bromide; [572-09-8]



R = acetyl-

$C_{14}H_{19}Br_1O_9$  (411.20). Solid. MP: 85°C. Decomposed by water. The commercial product is the D-(+)-enantiomer.

## Production

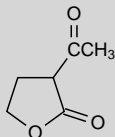
- pentaacetylglucose + hydrobromic acid (hydrolysis/ alcohol bromination)

## Derivatives

auranofin  
aurothioglucose

# 3-acetobutyrolactone

2-acetyl-1,4-butyrolactone;  $\alpha$ -acetobutyrolactone; ABL; acetylbutyrolactone; [517-23-7]



$C_6H_8O_3$  (128.13).

## Production

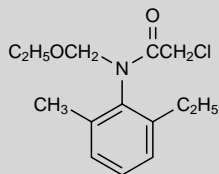
- ethyl acetoacetate + ethylene oxide (epoxidation)

## Derivatives

4-amino-1-diethylaminopentane  
cyclopropyl methyl ketone  
5-(2-hydroxyethyl)-4-methylthiazole  
paliperidone  
risperidone  
thiamine

# acetochlor

2-chloro-*N*-(ethoxyethyl)-6'-ethylacet-*o*-toluidide; [34256-82-1]



$C_{14}H_{20}Cl_1N_1O_2$  (269.77).

## Uses

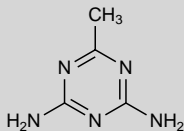
herbicide

## Production

- 2-ethyl-6-methylaniline + formaldehyde + ethanol + chloroacetyl chloride (alkoxymethylation/amide formation)

# acetoguanamine

2,4-diamino-6-methyl-1,3,5-triazine; [542-02-9]; 208-796-3 (EC)



C<sub>4</sub>H<sub>7</sub>N<sub>5</sub> (125.13). Solid. MP: 228°C. d: 1.42 kg/l. Slightly soluble in water. Soluble in oxygenated solvents.

## Uses

chemically-resistant/improved-solubility amino resin comonomer

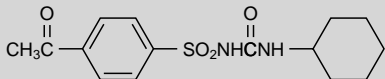
## Production

- acetonitrile + dicyandiamide (cyclocondensation)



# aceto hexamide

4-acetyl-*N*-[(cyclohexylamino)carbonyl]benzenesulfonamide; *N*-(*p*-acetylbenzenesulfonyl)-*N'*-cyclohexylurea;  
[968-81-0]



$C_{15}H_{20}N_2O_4S_1$  (324.40).

## Uses

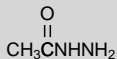
diabetes mellitus drug

## Production

- *p*-aminoacetophenone + sulfur dioxide, pure + ammonia + cyclohexyl isocyanate (diazotisation/sulfonate formation/sulfonamide formation/isocyanate addition)

# acetohydrazide

acetyl hydrazine; [1068-57-1]; 213-948-7 (EC)



$\text{C}_2\text{H}_6\text{N}_2\text{O}_1$  (74.08). Solid. MP: 63–66°C. Soluble in water.

## Production

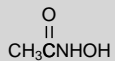
- acetic anhydride + hydrazine (amide formation)

## Derivatives

amicarbazono  
1,1-dimethylhydrazine  
metamitron  
2-methyl-5-mercapto-1,3,4-thiadiazole  
pymetrozine  
raltegravir  
sulfamethizole  
tiadinil  
triazolam

# acetoxyhydroxamic acid

*N*-hydroxyacetamide; [546-88-3]



$\text{C}_2\text{H}_5\text{N}_1\text{O}_2$  (75.07).

## Uses

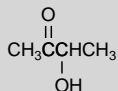
veterinary urinary tract treatment drug

## Production

- acetic anhydride + hydroxylamine sulfate (amide formation)

# acetoin

3-hydroxybutan-2-one; acetylmethylcarbinol; [513-86-0]



C<sub>4</sub>H<sub>8</sub>O<sub>2</sub> (88.11). Colourless liquid with a pleasant odour. BP: 148°C. MP: 15°C. d: 0.99 kg/l (20°C). Miscible with water and alcohol. Forms a solid dimer on standing which dissociates on heating.

## Uses

flavouring ingredient (margarine)

## Production

- methyl ethyl ketone (electrolytic oxidation; byproduct of diacetyl production)

## Derivatives

4-chloromethyl-5-methyl-1,3-dioxol-2-one  
dimethipin  
sulfamoxole

# acetone

2-propanone; dimethyl ketone; DMK; [67-64-1]



$\text{C}_3\text{H}_6\text{O}_1$  (58.08). Colourless, volatile liquid with a characteristic, ethereal odour. BP: 56°C. d: 0.79 kg/l (20°C). Miscible with water as well as most organic solvents and oils. Flash point: -9°C (OC).

## Uses

solvent (acetylene storage); solvent (varnish, lacquers, printing inks, adhesives, cellulose resins); essential oil extraction solvent; alcohol group protection reagent

## Production

- isopropanol (vapour-phase dehydrogenation)
- propylene oxide (isomerisation; byproduct of allyl alcohol production)
- cumene (liquid-phase oxidation/acid-catalysed hydrolysis; coproduced with phenol)
- toluene + propylene (Friedel-Crafts alkylation/liquid-phase oxidation/acid-catalysed hydrolysis; coproduced with *m/p*-cresol)
- *m*-diisopropylbenzene (liquid-phase oxidation/acid-catalysed hydrolysis; coproduced with resorcinol)
- *p*-diisopropylbenzene (liquid-phase oxidation/acid-catalysed hydrolysis; coproduced with hydroquinone)
- oxygenates, Fischer-Tropsch, mixed (fractionation; coproduced with methanol/acetaldehyde/ethanol/acetic acid/isopropanol/*n*-propanol/methyl ethyl ketone/*n*-butanol)
- naphtha, heavy (liquid-phase oxidation process; coproduced with formic acid/acetic acid/methyl ethyl ketone/propionic acid)
- isopropanol + oxygen (Shell autooxidation process; coproduced with hydrogen peroxide)

## Derivatives

acencoumarol

# acetone

2-propanone; dimethyl ketone; DMK; [67-64-1]

## Derivatives (Continued)

acetone cyanohydrin  
acetone-diphenylamine condensates  
alitame  
amisulbrom  
2,2'-azobisisobutyronitrile  
benzylideneacetone  
bezafibrate  
bisphenol A  
bromoform  
butoxydim  
*t*-butyl (3R,5S)-6-hydroxy-3,5-*O*-isopropylidene-3,5-dihydroxyhexanoate  
ciprofibrate  
citraxanthin  
clofibrate  
cyanazine  
cycloxydim  
diacetone alcohol  
2,2-di-(*t*-amylperoxy)propane  
diisobutyl ketone  
dikegulac-sodium  
2,2-dimethoxypropane  
dimethyl benzyl carbinol  
dimethyl hexynediol  
5,5-dimethylhydantoin  
dobutamine  
enestroburin

# acetone

2-propanone; dimethyl ketone; DMK; [67-64-1]

## Derivatives (Continued)

6-ethoxy-2,2,4-trimethyl-1,2-dihydroquinoline  
5-(2-ethylthiopropyl)-1,3-cyclohexanedione  
etretinate  
fenofibrate  
flufenacet  
fluvastatin  
furilazole  
glafenine  
hetacillin  
hydramethylnon  
4-hydroxybenzylacetone  
iodoform  
iproniazid  
isocarboxazid  
isophorone  
isophytol  
isopropanol  
isopropenyl acetate  
isopropylidene-D-glyceraldehyde  
isopropylidene-D-glycerol  
*N*-isopropyl-*N'*-phenyl-*p*-phenylenediamine  
2,6-lutidine  
Meldrum's acid  
methyl *n*-amyl ketone  
methylbutynol  
methylglyoxal dimethyl acetal  
 $\alpha$ -methylheptenone

# acetone

2-propanone; dimethyl ketone; DMK; [67-64-1]

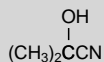
## Derivatives (Continued)

$\beta$ -methylheptenone  
2-methylindole  
methyl isoamyl ketone  
methyl isobutyl ketone  
methyl vinyl ketone  
nabumetone  
phorone  
 $\alpha$ -picoline  
probutol  
profoxydim  
prohexadione-calcium  
propachlor  
propaquizafoxop  
propylene  
pseudoionone  
sulfadiazamide  
tepraloxym  
topiramate  
tralkoxydim  
2,2,4-trimethyl-1,2-dihydroquinoline, polymeric  
trinexapac-ethyl



# acetone cyanohydrin

2-hydroxy-2-methylpropanenitrile; ACH;  $\alpha$ -hydroxyisobutyronitrile; [75-86-5]



$\text{C}_4\text{H}_7\text{N}_1\text{O}_1$  (85.10). Colourless liquid. BP: 82°C. FP: -19°C. d: 0.93 kg/l (20°C). Miscible with water and most organic solvents.

## Production

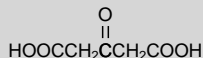
- acetone + hydrogen cyanide (cyanohydrin formation)

## Derivatives

butafenacil  
2,3,5-collidine  
lercanidipine  
methacrylamide sulfate  
methacrylonitrile  
methyl methacrylate  
raltegravir  
trimethadione  
valnemulin

# acetonedicarboxylic acid

$\beta$ -ketoglutaric acid; acetone-1,3-dicarboxylic acid; [542-05-2]



$\text{C}_5\text{H}_6\text{O}_5$  (146.10). White, crystalline powder. MP: 135°C with decomposition. Soluble in water and alcohol. Insoluble in chlorinated and aromatic solvents.

## Production

- carbon disulfide + ethyl acetate (thiocarbonylation/hydrolysis)
- methyl  $\gamma$ -chloroacetoacetate + hydrogen cyanide (cyanidation/hydrolysis)

## Derivatives

dolasetron  
tolmetin

# acetone-diphenylamine condensates

ADPA; diphenylamine-acetone condensates

Mixed product containing quinoline and aromatic amine derivatives.

## Uses

antioxidant (rubber)

## Production

- diphenylamine + acetone (carbonyl condensation)

# acetonitrile

methyl cyanide; [75-05-8]

CH<sub>3</sub>CN

C<sub>2</sub>H<sub>3</sub>N<sub>1</sub> (41.05). Colourless liquid with an ethereal odour. BP: 81°C. MP: -45°C. d: 0.79 kg/l (15°C). Miscible with water, oxygenated and chlorinated solvents. Immiscible with aliphatic hydrocarbons.

## Uses

selective solvent (butadiene extraction); process solvent

## Production

- propylene + ammonia (ammoxidation; byproduct of acrylonitrile production)

## Derivatives

acetamide hydrochloride  
acetamidiprid  
acetoguanamine  
amantadine  
β-aminocrotonitrile  
(2*S*,3*S*,5*S*)-2-amino-3-hydroxy-5-(*t*-butyloxycarbonylamino)-1,6-diphenylhexane  
(1*S*,2*R*)-1-amino-2-indanol  
2-amino-4-methoxy-6-methyltriazine  
*N*,*O*-bis(trimethylsilyl)acetamide  
butorphanol  
carfentrazone-ethyl  
3,3-diethoxypropionitrile  
3,4-dihydroxy-ω-chloroacetophenone  
3,3-dimethoxypropionitrile  
drotaverine  
geranonitrile  
halofuginone  
homoveratric acid  
isoxaben  
malononitrile  
memantine

# acetonitrile

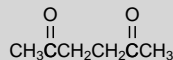
methyl cyanide; [75-05-8]

## Derivatives (Continued)

sulfaisodimidine  
sulfametomidine  
sulfentrazone  
thifluzamide  
triethyl orthoacetate  
trimethyl orthoacetate

# acetylacetone

2,5-hexanedione; hexane-2,5-dione; [110-13-4]



$\text{C}_6\text{H}_{10}\text{O}_2$  (114.14). Colourless liquid. BP: 190–192°C. MP: -9°C. d: 0.97 kg/l (20°C). Miscible with water and oxygenated solvents.

## Production

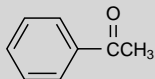
- methyl acetoacetate (oxidative coupling/decarboxylation)

## Derivatives

glisoxepide  
3-methyl-2-hydroxy-2-cyclopentenone  
pyrvinium pamoate

# acetophenone

acetylbenzene; [98-86-2]



$C_8H_8O_1$  (120.15). Colourless liquid with a characteristic odour. MP: 19°C. Slightly soluble in water. Soluble in organic solvents. Soluble in hydrocarbon and oxygenated solvents. Insoluble in water.

## Uses

fragrance ingredient (detergent, technical products)

## Production

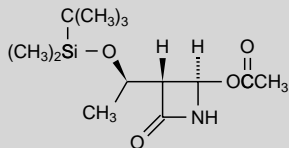
- cumene (liquid-phase oxidation/acid-catalysed hydrolysis; byproduct of acetone/phenol production)

## Derivatives

$\alpha$ -chloroacetophenone  
dibenzoylmethane  
2,2-diethoxyacetophenone  
3,5-dihydroxyacetophenone  
disodium 4,4'-bis(4-phenyl-1,2,3-triazol-2-yl)stilbene-2,2'-disulfonate  
ethyl methylphenylglycidate  
fenamidone  
fendiline  
fluoxetine  
isopropyl dibenzoyl methane  
mesuximide  
(*R*)- $\alpha$ -methylbenzylamine  
(*S*)- $\alpha$ -methylbenzylamine  
*m*-nitroacetophenone  
 $\beta$ -phenylindole  
procyclidine  
pyrazoxyfen  
stearoylbzoylmethane  
tilidine  
trihexyphenidyl

# (3*R*,4*R*)-4-acetoxy-3-[(*R*)-1-(*t*-butyldimethylsilyloxy)ethyl]-2-azetidinone

4-acetoxyazetidin-2-one; 4-ABA; 4-AA; 4-AOSA; [76855-69-1]



C<sub>13</sub>H<sub>25</sub>N<sub>1</sub>O<sub>4</sub>Si<sub>1</sub> (287.43).

## Production

- methyl D-β-hydroxybutyrate + *t*-butyldimethylchlorosilane + chlorosulfonyl isocyanate (O-protection/enantiospecific hydrogenation/O-protection/cycloaddition/O-acetylation)
- benzoyl chloride + ammonia + formaldehyde + methyl acetoacetate + *t*-butyldimethylchlorosilane (amide formation/chloromethylation/dehydrochlorination/enantiospecific catalytic hydrogenation/amide hydrolysis/cyclisation/O-protection/catalytic peroxidation/O-acetylation)

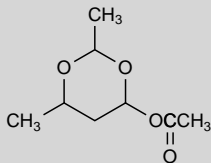
## Derivatives

(3*S*,4*S*)-3-[(*R*)-1-(*t*-butyldimethylsilyloxy)ethyl]-4-(carboxyethyl)-2-azetidinone  
imipenem



## 6-acetoxy-2,4-dimethyl-1,3-dioxane

2,6-dimethyl-1,3-dioxan-4-yl acetate; dimethoxane; [828-00-2]; 212-579-9 (EC)



$C_8H_{14}O_4$  (174.19).

### Uses

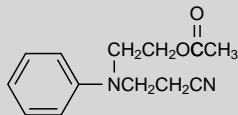
preservative (detergents, lubricants, paint)

### Production

- acetaldehyde + acetic anhydride (aldol condensation/ acetal formation/O-acetylation)

# ***N*-(2-acetoxyethyl)-*N*-(2-cyanoethyl)aniline**

3-(*N*-2-acetoxyethylanilino)propionitrile; 3-[(2-acetoxyethyl)phenylamino]propionitrile; [22031-33-0]



$C_{13}H_{16}N_2O_2$  (232.28). Liquid. BP: 202–258°C (4.0 kPa).

## **Production**

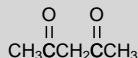
- acetic acid + *N*-(2-cyanoethyl)-*N*-(2-hydroxyethyl)aniline (ester formation)

## **Derivatives**

Disperse Orange 30  
Disperse Orange 31  
Disperse Red 72  
Disperse Red 136  
Disperse Red 137  
Disperse Red 177

# acetylacetone

2,4-pentanedione; ACAC; pentan-2,4-dione; [123-54-6]



C<sub>5</sub>H<sub>8</sub>O<sub>2</sub> (100.12). Colourless or yellowish liquid. MP: -23°C. BP: 139°C. d: 0.97 kg/l (20°C).

## Uses

solvent (cellulose acetate); extraction solvent (mineral processing); metal deactivator (lubricants, fuel, anticorrosion preparations); paint dryer

## Production

- isopropenyl acetate (rearrangement)
- ethyl acetoacetate + ketene (addition/decarboxylation)

## Derivatives

acetylacetone peroxide  
Acid Orange 165  
cobalt acetylacetonate  
4,6-dimethyl-2-hydroxypyrimidine  
ferric acetylacetonate  
*N*-hydroxymethyl-3,5-dimethylpyrazole  
nickel acetylacetonate  
pyrimethanil  
sulfadimidine  
sulfometuron-methyl

# acetylacetone peroxide

2,4-pentanedione peroxide; Luperox 224 (Arkema); [37187-22-7]

Mixed product containing  $\alpha$ -hydroxy- and  $\alpha$ -peroxyhydroperoxides. Commercial grades have 4% active oxygen.

## Uses

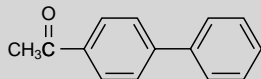
unsaturated polyester resin crosslinking agent

## Production

- acetylacetone + hydrogen peroxide (peroxidation)

# 4-acetylbiphenyl

4'-phenylacetophenone; [92-91-1]



$C_{14}H_{12}O_1$  (196.24). Solid. MP: 117–119°C. BP: 325°C.  
Insoluble in water. Soluble in oxygenated solvents.

## Production

- biphenyl + acetyl chloride (Friedel-Crafts acylation)

## Derivatives

biphenyl-4-carboxylic acid  
bromadiolone

# acetyl chloride

[75-36-5]

CH<sub>3</sub>COCl

C<sub>2</sub>H<sub>3</sub>Cl<sub>1</sub>O<sub>1</sub> (78.50). Colourless liquid with a pungent odour. BP: 52°C. MP: -113°C. d: 1.11 kg/l (20°C). Fumes in moist air. Hydrolysed by water and alcohol. Soluble in oxygenated, chlorinated and aromatic solvents. Acetyl chloride is often produced *in situ* by reaction of acetic anhydride with hydrochloric acid.

## Uses

esterification/acetylation/acid chlorination catalyst

## Production

- sodium acetate + sulfur dioxide, pure + chlorine (acid chloride formation)
- acetic acid + benzotrichloride (acid chloride formation; coproduced with benzoyl chloride)

## Derivatives

acepromazine  
4-acetylbiphenyl  
4-acetyl-1,1-dimethyl-6-*t*-butylindane  
6-acetyl-1,1,2,3,3,5-hexamethylindane  
6-acetyl-1,1,2,4,4,7-hexamethyltetralin  
6-aminoveratric acid  
atovaquone  
beryllium  
besifloxacin  
*t*-butyl peroxyacetate  
2-chloroacetophenone  
4-chloroacetophenone  
2,4-dichloroacetophenone  
2,4-dichloro-5-fluoroacetophenone  
efomedoterol  
etymemazine  
famoxadone  
fluconazole  
flurbiprofen  
indole-3-carboxylic acid

# acetyl chloride

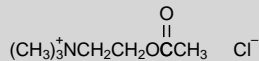
[75-36-5]

## Derivatives (Continued)

*p*-isobutylacetophenone  
metaflumizone  
3-methoxy- $\alpha$ -picoline  
methyl  $\beta$ -naphthyl ketone  
nebivolol  
oxolinic acid  
penflufen  
pyribencarb  
tazarotene  
tebufenozide  
tefuryltrione  
tembotrione  
trifloxystrobin  
Vat Blue 66

# acetylcholine chloride

[60-31-1]



$\text{C}_7\text{H}_{16}\text{Cl}_1\text{N}_1\text{O}_2$  (181.66). Yellowish, crystalline powder.  
MP: 149–152°C. Solubility in water: 600 g/l (20°C).

## Uses

ophthalmic surgery drug

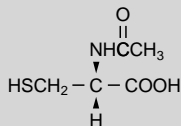
## Production

- choline chloride + acetic acid (N-acetylation)



# N-acetyl-L-cysteine

acetylcysteine; L-2-acetamido-3-mercaptopropionic acid; [616-91-1]



$\text{C}_5\text{H}_9\text{N}_1\text{O}_3\text{S}_1$  (163.19).

## Uses

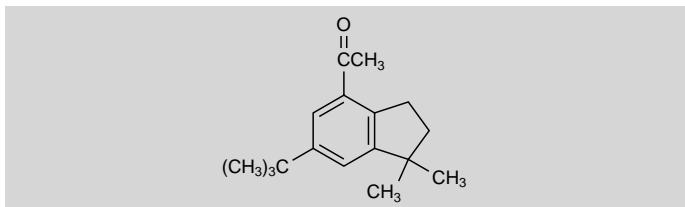
mucolytic/tear deficiency drug

## Production

- L-cysteine + acetic anhydride (amide formation)

# 4-acetyl-1,1-dimethyl-6-*t*-butylindane

ADBI; Celestolide (IFF); Crysolide (Givaudan); [13171-00-1]



$C_{17}H_{24}O_1$  (244.37). Solid with a musk-like odour. MP: 77°C.

## Uses

fragrance ingredient

## Production

- *t*-butylbenzene + isoprene + acetyl chloride (acid-catalysed cyclisation/Friedel-Crafts acylation)

# acetylene

ethyne; [74-86-2]



C<sub>2</sub>H<sub>2</sub> (26.04). Colourless gas with an unpleasant odour. Solid sublimes at temperatures above -81°C. Relative density: 0.90 (gas, air=1). Slightly soluble in water. Supplied for welding purposes in cylinders as a solution in acetone or DMF held in a porous calcium silicate matrix. For other purposes the product is used *in situ*.

## Uses

welding gas

## Production

- natural gas + *n*-butane (Huels electric arc process; coproduced with ethylene)
- calcium carbide (hydrolysis)
- naphtha, heavy/gasoline, dearomatised/gasoline, natural (steam cracking; byproduct of ethylene/propylene/C<sub>4</sub>-stream, steam-cracked/gasoline, pyrolysis/pyrolysis tar production)
- gas oil, heavy/gas oil, vacuum/gas oil, light (steam cracking; byproduct of ethylene/propylene/C<sub>4</sub>-stream, steam-cracked/gasoline, pyrolysis/pyrolysis tar production)
- raffinate I, hydrogenated/liquified petroleum gas (steam cracking; byproduct of ethylene/propylene/C<sub>4</sub>-stream, steam-cracked/gasoline, pyrolysis/pyrolysis tar production)
- natural gas + oxygen (SBA process; coproduced with synthesis gas)
- naphtha, heavy/natural gas + oxygen (Montecatini autothermic process; coproduced with synthesis gas)
- natural gas + oxygen (BASF partial combustion process; coproduced with synthesis gas)

## Derivatives

acetaldehyde *n*-propyl phenethyl diacetal

# acetylene

ethyne; [74-86-2]

## Derivatives (Continued)

acetylene black  
buprenorphine  
*n*-butyl vinyl ether  
1,4-butyndiol  
1-butyne-3-ol  
canrenone  
 $\beta$ -carotene  
chloroprene  
C<sub>15</sub> triphenylphosphonium chloride  
dehydrolinalool  
dichloromethylvinylsilane  
diethylene glycol divinyl ether  
dimethyl hexynediol  
dimethyl hexynol  
dimethyl octynediol  
drospirenone  
empenthrin  
erlotinib  
ethinylestradiol  
ethisterone  
ethylene dichloride  
ethyl octynol  
ethyl vinyl ether  
ethynyl cyclohexanol  
etonogestrel  
etretinate  
geranylgeraniol

# acetylene

ethyne; [74-86-2]

## Derivatives (Continued)

3-hexenol  
2,5-hexynediol  
4-hydroxybutyl vinyl ether  
isobutyl vinyl ether  
isodecaprenol  
isophytol  
japonilure  
levonorgestrel  
mestranol  
methohexital  
3-methoxygestra-2,5-diene-17-one  
methylacetylene  
methylbutynol  
methyl 3-formylcrotonate  
methyl 2-nonynoate  
14-methyloctadecene  
methyl 2-octynoate  
2-methylpent-2-en-4-yn-1-al diethyl acetal  
methyl pentenynol  
methylpentynol  
*N*-methyl-*N*-vinylacetamide  
methyl vinyl ether  
mivacurium chloride  
nerolidol  
norethisterone  
1-octen-3-ol  
sodium vinyl sulfonate

# acetylene

ethyne; [74-86-2]

## Derivatives (Continued)

stearyl vinyl ether  
tetrabromoethane  
tetramethyl decynediol  
trichloroethylene  
vinyl acetate  
vinyl bromide  
*N*-vinylcaprolactam  
*N*-vinylcarbazole  
vinyl chloride  
vinyl fluoride  
*N*-vinylimidazole  
vinyl neodecanoate  
vinyl propionate  
*N*-vinyl-2-pyrrolidone  
vinyltrichlorosilane

# acetylene black

carbon black; [1333-86-4]

Black solid. Particles are platelets 40 nm in diameter with a specific surface area of  $\sim 65 \text{ m}^2/\text{g}$ .

## Uses

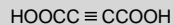
electrically-conductive filler (rubber heater pads and tapes); antistatic rubber/plastics filler (conveyor belts, drives, shoe soles); battery electrodes

## Production

- acetylene (acetylene black process)

# acetylenedicarboxylic acid

butyne-1,4-dioic acid; [142-45-0]; 205-536-0 (EC)



$\text{C}_4\text{H}_2\text{O}_4$  (114.06). Solid. MP: 185–190°C with decomposition. Soluble in water.

## Production

- 1,4-butyne-1,3-diol (electrolytic oxidation)

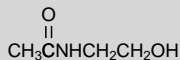
## Derivatives

fluoroimide  
nedocromil  
raltegravir



# N-acetyethanolamine

N-2-hydroxyethylacetamide; [142-26-7]



$\text{C}_4\text{H}_9\text{N}_1\text{O}_2$  (103.12). Liquid or solid. FP: 16°C. Decomposes on heating. Miscible with water.

## Production

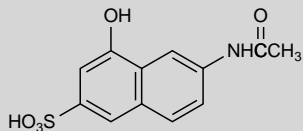
- acetic anhydride + monoethanolamine (amide formation)

## Derivatives

1-acetyl-2-imidazolidinone  
amlodipine

# acetyl-gamma acid

[6361-41-7]; 228-836-3 (EC)



$C_{12}H_{11}N_1O_5S_1$  (281.28).

## Uses

dyestuffs intermediate

## Production

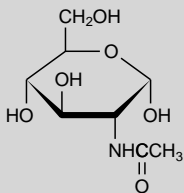
- amino-G acid + acetic anhydride (N-acetylation/alkali fusion)

## Derivatives

Reactive Orange 7  
Reactive Orange 16

# N-acetylglucosamine

2-acetamido-2-deoxy-β-D-glucan; NAG; [7512-17-6]



$C_8H_{15}N_1O_6$  (221.21). The  $\alpha$ -epimer is shown in the structure.

## Production

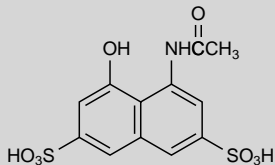
- glucosamine hydrochloride + acetic anhydride (N-acetylation)

## Derivatives

*N*-acetyl-D-mannosamine  
*N*-acetylneuraminic acid

## N-acetyl-H acid

1-acetamido-8-naphthol-3,6-disulfonic acid; 8-acetamido-1-hydroxynaphthalene-3,6-disulfonic acid; [16698-16-1]; [134-34-9]; 205-139-2 (EC); 240-746-6 (EC)



$C_{12}H_{11}N_1O_8S_2$  (361.35).

### Production

- acetic anhydride + H acid (amide formation)

### Derivatives

Acid Red 1  
Acid Red 35  
Acid Red 138  
Acid Violet 7  
Reactive Blue 13  
Reactive Violet 4  
Reactive Violet 5