

Table 1. Acids: Alphabetical Order

| Class | Acid                             | $M_r$   | $pK_{a1}$ | $pK_{a2}$ | $pK_{a3}$ | ADI up to [mg/kg] | GRAS Status |      |      |   |
|-------|----------------------------------|---------|-----------|-----------|-----------|-------------------|-------------|------|------|---|
| 1     | Acetic acid                      | 60.05   | 4.756     | A         |           | n.s.              | +           |      |      |   |
| 3     | Acetic acid, 2,2-dichloro-       | 128.95  | 1.35      | A         |           |                   |             |      |      |   |
| 1     | Adipic acid                      | 146.14  | 4.44      | A         | 5.44      | A                 | 5           | +    |      |   |
| 2     | Alginic acid                     | 240 000 | 2.4       | A         |           |                   | n.s.        | +    |      |   |
| 1     | L-Ascorbic acid                  | 176.13  | 4.17      | A         | 11.57     | A                 |             | +    |      |   |
| 1     | L-Aspartic acid                  | 133.11  | 1.88      | A         | 3.65      | A                 | 9.60        | B    |      |   |
| 2     | Benzenesulfonic acid             | 158.18  | 0.7       | A         |           |                   |             |      |      |   |
| 2     | Benzoic acid                     | 122.12  | 4.19      | A         |           |                   |             | +    |      |   |
| 3     | Benzoic acid, 4-acetamido-       | 179.18  | 4.3       | A         |           |                   |             |      |      |   |
| 2     | (+)-Camphoric acid               | 200.24  | 4.716     | A         | 5.83      | A                 |             |      |      |   |
| 3     | (+)-Camphor-10-sulfonic acid     | 232.29  | 2.17      | A         |           |                   |             |      |      |   |
| 1     | Capric acid (decanoic acid)      | 172.27  | 4.9       | A         |           |                   | n.s.        |      |      |   |
| 3     | Caproic acid (hexanoic acid)     | 116.16  | 4.8       | A         |           |                   |             |      |      |   |
| 2     | Caprylic acid (octanoic acid)    | 144.22  | 4.91      | A         |           |                   | n.s.        | +    |      |   |
| 1     | Carbonic acid                    | 44.01   | 6.46      | A         | 10.3      | A                 |             | n.s. | +    |   |
| 3     | Cinnamic acid                    | 148.16  | 4.404     | A         |           |                   |             |      |      |   |
| 1     | Citric acid                      | 192.13  | 3.128     | A         | 4.761     | A                 | 6.396       | A    | n.s. | + |
| 2     | Cyclamic acid                    | 179.24  | -2.01     | A         |           |                   |             |      |      |   |
|       | Decanoic acid (see capric acid)  |         |           |           |           |                   |             |      |      |   |
| 2     | Dodecylsulfuric acid             | 266.40  | -0.09     | A         |           |                   |             |      |      |   |
| 2     | Ethane-1,2-disulfonic acid       | 190.20  | -2.1      | A         | -1.5      | A                 |             |      |      |   |
| 2     | Ethanesulfonic acid              | 110.13  | 2.05      | A         |           |                   |             |      |      |   |
| 2     | Ethanesulfonic acid, 2-hydroxy-  | 126.13  | 1.66      | A         |           |                   |             |      |      |   |
| 3     | Formic acid                      | 46.02   | 3.75      | A         |           |                   |             |      |      |   |
| 1     | Fumaric acid                     | 116.08  | 3.03      | A         | 4.38      | A                 |             |      | 6    |   |
| 1     | Galactaric acid                  | 210.14  | 3.08      | A         | 3.63      | A                 |             |      |      |   |
| 2     | Gentisic acid                    | 154.12  | 2.93      | A         |           |                   |             |      |      |   |
| 1     | D-Glucoheptonic acid             | 226.18  | 3.3       | A         |           |                   |             |      |      |   |
| 1     | D-Gluconic acid                  | 196.16  | 3.76      | A         |           |                   |             |      | 50   | # |
| 1     | D-Glucuronic acid                | 194.14  | 3.18      | A         |           |                   |             |      |      |   |
| 1     | Glutamic acid                    | 147.13  | 2.19      | A         | 4.25      | A                 | 9.67        | B    |      | + |
| 1     | Glutaric acid                    | 132.12  | 4.34      | A         | 5.27      | A                 |             |      |      |   |
| 2     | Glutaric acid, 2-oxo-            | 146.10  | 2.7       | A         | 4.5       | A                 |             |      |      |   |
| 1     | Glycerophosphoric acid           | 172.08  | 1.47      | A         | 6.19      | A                 |             |      |      |   |
| 1     | Glycolic acid                    | 76.05   | 3.28      | A         |           |                   |             |      |      |   |
|       | Hexanoic acid (see caproic acid) |         |           |           |           |                   |             |      |      |   |
| 1     | Hippuric acid                    | 179.17  | 3.55      | A         |           |                   |             |      |      |   |

Table 1 (cont.)

| Class | Acid                                   | $M_r$  | $pK_{a1}$ | $pK_{a2}$ | $pK_{a3}$ | ADI up to [mg/kg] | GRAS Status |      |   |
|-------|--|--------|-----------|-----------|-----------|-------------------|-------------|------|---|
| 3     | Hydrobromic acid                       | 80.92  | <-6       | A         |           |                   |             |      |   |
| 1     | Hydrochloric acid                      | 36.46  | -6        | A         |           |                   | n.s.        | +    |   |
| 2     | Isobutyric acid                        | 88.11  | 4.86      | A         |           |                   |             |      |   |
| 1     | DL-Lactic acid                         | 90.08  | 3.86      | A         |           |                   |             |      | + |
| 2     | Lactobionic acid                       | 358.30 | 3.2       | A         |           |                   |             |      |   |
| 1     | Lauric acid                            | 200.32 | 4.9       | A         |           |                   |             | n.s. |   |
| 1     | Maleic acid                            | 116.08 | 1.92      | A         | 6.23      | A                 |             |      |   |
| 1     | (-)-L-Malic acid                       | 134.09 | 3.459     | A         | 5.097     | A                 |             | n.s. | + |
| 2     | Malonic acid                           | 104.06 | 2.826     | A         | 5.696     | A                 |             |      |   |
| 3     | DL-Mandelic acid                       | 152.15 | 3.372     | A         |           |                   |             |      |   |
| 2     | Methanesulfonic acid                   | 96.10  | -1.2      | A         |           |                   |             |      |   |
|       | Mucic acid (see galactaric acid)       |        |           |           |           |                   |             |      |   |
| 2     | Naphthalene-1,5-disulfonic acid        | 332.26 | -3.37     | A         | -2.64     | A                 |             |      |   |
| 2     | Naphthalene-2-sulfonic acid            | 208.24 | 0.17      | A         |           |                   |             |      |   |
| 2     | 2-Naphthoic acid, 1-hydroxy-           | 188.17 | 2.7       | A         | 13.5      | A                 |             |      |   |
| 2     | Nicotinic acid                         | 123.11 | 4.85      | A         | 2.07      | B                 |             |      | + |
| 3     | Nitric Acid                            | 63.02  | -1.32     | A         |           |                   |             |      |   |
|       | Octanoic acid (see caprylic acid)      |        |           |           |           |                   |             |      |   |
| 2     | Oleic acid                             | 282.45 | ca. 4     | A         |           |                   |             |      |   |
| 2     | Orotic acid                            | 156.10 | 5.85      | A         | 8.95      | A                 |             |      |   |
| 2     | Oxalic acid                            | 90.04  | 1.271     | A         | 4.266     | A                 |             |      |   |
| 1     | Palmitic acid                          | 256.42 | 4.9       | A         |           |                   |             | n.s. |   |
| 2     | Pamoic acid (embonic acid)             | 388.38 | 2.51      | A         | 3.1       | A                 |             |      |   |
| 1     | Phosphoric acid                        | 98.00  | 1.96      | A         | 7.12      | A                 | 12.32       | A    | + |
| 2     | Propionic acid                         | 74.08  | 4.87      | A         |           |                   |             | n.s. | + |
| 2     | (-)-L-Pyroglutamic acid                | 129.11 | 3.32      | A         |           |                   |             |      |   |
| 3     | Salicylic acid                         | 138.12 | 2.97      | A         | 13.82     | A                 |             |      |   |
| 3     | Salicylic acid, 4-amino-               | 153.14 | 3.25      | A         | 10        | A                 | 3.5         | B    |   |
| 1     | Sebacic acid                           | 202.25 | 4.59      | A         | 5.59      | A                 |             |      |   |
| 1     | Stearic acid                           | 284.49 | 4.9       | A         |           |                   |             | n.s. | + |
| 1     | Succinic acid                          | 118.09 | 4.207     | A         | 5.635     | A                 |             | n.s. | + |
| 1     | Sulfuric acid                          | 98.08  | -3        | A         | 1.92      | A                 |             | n.s. | + |
| 1     | (+)-L-Tartaric acid                    | 150.09 | 3.02      | A         | 4.36      | A                 |             |      | + |
| 1     | Thiocyanic acid                        | 59.09  | -1.33     | A         |           |                   |             |      |   |
| 2     | p-Toluenesulfonic acid                 | 172.21 | -1.34     | A         |           |                   |             |      |   |
| 3     | Undecylenic acid (undec-10-enoic acid) | 184.27 | 4.9       | A         |           |                   |             |      |   |

Table 2. Acids: Sorted by Increasing  $pK_{a1}$  Value

| Class | Acid                              | $M_r$   | $pK_{a1}$ | $pK_{a2}$ | $pK_{a3}$ | ADI<br>up to<br>[mg/kg] | GRAS<br>Status |
|-------|-----------------------------------|---------|-----------|-----------|-----------|-------------------------|----------------|
|       | Decanoic acid (see capric acid)   |         |           |           |           |                         |                |
|       | Hexanoic acid (see caproic acid)  |         |           |           |           |                         |                |
|       | Mucic acid (see galactaric acid)  |         |           |           |           |                         |                |
|       | Octanoic acid (see caprylic acid) |         |           |           |           |                         |                |
| 3     | Hydrobromic acid                  | 80.92   | < -6      | A         |           |                         |                |
| 1     | Hydrochloric acid                 | 36.46   | -6        | A         |           | n.s.                    | +              |
| 2     | Naphthalene-1,5-disulfonic acid   | 332.26  | -3.37     | A         | -2.64     | A                       |                |
| 1     | Sulfuric acid                     | 98.08   | -3        | A         | 1.92      | A                       | n.s.           |
| 2     | Ethane-1,2-disulfonic acid        | 190.20  | -2.1      | A         | -1.5      | A                       |                |
| 2     | Cyclamic acid                     | 179.24  | -2.01     | A         |           |                         |                |
| 2     | <i>p</i> -Toluenesulfonic acid    | 172.21  | -1.34     | A         |           |                         |                |
| 1     | Thiocyanic acid                   | 59.09   | -1.33     | A         |           |                         |                |
| 3     | Nitric Acid                       | 63.02   | -1.32     | A         |           |                         |                |
| 2     | Methanesulfonic acid              | 96.10   | -1.2      | A         |           |                         |                |
| 2     | Dodecylsulfuric acid              | 266.40  | -0.09     | A         |           |                         |                |
| 2     | Naphthalene-2-sulfonic acid       | 208.24  | 0.17      | A         |           |                         |                |
| 2     | Benzenesulfonic acid              | 158.18  | 0.7       | A         |           |                         |                |
| 2     | Oxalic acid                       | 90.04   | 1.271     | A         | 4.266     | A                       |                |
| 3     | Acetic acid, 2,2-dichloro-        | 128.95  | 1.35      | A         |           |                         |                |
| 1     | Glycerophosphoric acid            | 172.08  | 1.47      | A         | 6.19      | A                       |                |
| 2     | Ethanesulfonic acid, 2-hydroxy-   | 126.13  | 1.66      | A         |           |                         |                |
| 1     | L-Aspartic acid                   | 133.11  | 1.88      | A         | 3.65      | A                       | 9.60 B         |
| 1     | Maleic acid                       | 116.08  | 1.92      | A         | 6.23      | A                       |                |
| 1     | Phosphoric acid                   | 98.00   | 1.96      | A         | 7.12      | A                       | 12.32 A        |
| 2     | Ethanesulfonic acid               | 110.13  | 2.05      | A         |           |                         |                |
| 3     | (+)-Camphor-10-sulfonic acid      | 232.29  | 2.17      | A         |           |                         |                |
| 1     | Glutamic acid                     | 147.13  | 2.19      | A         | 4.25      | A                       | 9.67 B         |
| 2     | Alginic acid                      | 240 000 | ≥ 2.4     | A         |           |                         | n.s.           |
| 2     | Pamoic acid (embonic acid)        | 388.38  | 2.51      | A         | 3.1       | A                       |                |
| 2     | Glutaric acid, 2-oxo-             | 146.10  | 2.7       | A         | 4.5       | A                       |                |
| 2     | 2-Naphthoic acid, 1-hydroxy-      | 188.17  | 2.7       | A         | 13.5      | A                       |                |
| 2     | Malonic acid                      | 104.06  | 2.826     | A         | 5.696     | A                       |                |
| 2     | Gentisic acid                     | 154.12  | 2.93      | A         |           |                         |                |
| 3     | Salicylic acid                    | 138.12  | 2.97      | A         | 13.82     | A                       |                |
| 1     | (+)-L-Tartaric acid               | 150.09  | 3.02      | A         | 4.36      | A                       |                |
| 1     | Fumaric acid                      | 116.08  | 3.03      | A         | 4.38      | A                       | 6              |

Table 2 (cont.)

| Class | Acid                                      | $M_r$  | $pK_{a1}$ | $pK_{a2}$ | $pK_{a3}$ | ADI<br>up to<br>[mg/kg] | GRAS<br>Status |
|-------|---|--------|-----------|-----------|-----------|-------------------------|----------------|
| 1     | Galactaric acid                           | 210.14 | 3.08      | A         | 3.63      | A                       |                |
| 1     | Citric acid                               | 192.13 | 3.128     | A         | 4.761     | A                       | 6.396 A        |
| 1     | D-Glucuronic acid                         | 194.14 | 3.18      | A         |           |                         | n.s.           |
| 2     | Lactobionic acid                          | 358.30 | 3.2       | A         |           |                         |                |
| 3     | Salicylic acid, 4-amino-                  | 153.14 | 3.25      | A         | 10        | A                       | 3.5 B          |
| 1     | Glycolic acid                             | 76.05  | 3.28      | A         |           |                         |                |
| 1     | D-Glucoheptonic acid                      | 226.18 | 3.3       | A         |           |                         |                |
| 2     | (-)-L-Pyroglutamic acid                   | 129.11 | 3.32      | A         |           |                         |                |
| 3     | DL-Mandelic acid                          | 152.15 | 3.372     | A         |           |                         |                |
| 1     | (-)-L-Malic acid                          | 134.09 | 3.459     | A         | 5.097     | A                       | n.s.           |
| 1     | Hippuric acid                             | 179.17 | 3.55      | A         |           |                         |                |
| 3     | Formic acid                               | 46.02  | 3.75      | A         |           |                         |                |
| 1     | D-Gluconic acid                           | 196.16 | 3.76      | A         |           |                         | 50             |
| 1     | DL-Lactic acid                            | 90.08  | 3.86      | A         |           |                         |                |
| 2     | Oleic acid                                | 282.45 | ca. 4     | A         |           |                         |                |
| 1     | L-Ascorbic acid                           | 176.13 | 4.17      | A         | 11.57     | A                       |                |
| 2     | Benzoic acid                              | 122.12 | 4.19      | A         |           |                         |                |
| 1     | Succinic acid                             | 118.09 | 4.207     | A         | 5.635     | A                       | n.s.           |
| 3     | Benzoic acid, 4-acetamido-                | 179.18 | 4.3       | A         |           |                         |                |
| 1     | Glutaric acid                             | 132.12 | 4.34      | A         | 5.27      | A                       |                |
| 3     | Cinnamic acid                             | 148.16 | 4.404     | A         |           |                         |                |
| 1     | Adipic acid                               | 146.14 | 4.44      | A         | 5.44      | A                       | 5              |
| 1     | Sebacic acid                              | 202.25 | 4.59      | A         | 5.59      | A                       |                |
| 2     | (+)-Camphoric acid                        | 200.24 | 4.716     | A         | 5.83      | A                       |                |
| 1     | Acetic acid                               | 60.05  | 4.756     | A         |           |                         | n.s.           |
| 3     | Caproic acid (hexanoic acid)              | 116.16 | 4.8       | A         |           |                         |                |
| 2     | Nicotinic acid                            | 123.11 | 4.85      | A         | 2.07      | B                       |                |
| 2     | Isobutyric acid                           | 88.11  | 4.86      | A         |           |                         |                |
| 2     | Propionic acid                            | 74.08  | 4.87      | A         |           |                         | n.s.           |
| 1     | Capric acid (decanoic acid)               | 172.27 | 4.9       | A         |           |                         | n.s.           |
| 1     | Lauric acid                               | 200.32 | 4.9       | A         |           |                         | n.s.           |
| 1     | Palmitic acid                             | 256.42 | 4.9       | A         |           |                         | n.s.           |
| 1     | Stearic acid                              | 284.49 | 4.9       | A         |           |                         | n.s.           |
| 3     | Undecylenic acid<br>(undec-10-enoic acid) | 184.27 | 4.9       | A         |           |                         |                |
| 2     | Caprylic acid (octanoic acid)             | 144.22 | 4.91      | A         |           |                         | n.s.           |
| 2     | Orotic acid                               | 156.10 | 5.85      | A         | 8.95      | A                       |                |
| 1     | Carbonic acid                             | 44.01  | 6.46      | A         | 10.3      | A                       | n.s.           |

Table 3. Acids: Sorted by Increasing Molecular Weight

| Class | Acid                              | $M_r$  | $pK_{a1}$ | $pK_{a2}$ | $pK_{a3}$ | ADI<br>up to<br>[mg/kg] | GRAS<br>Status |
|-------|-----------------------------------|--------|-----------|-----------|-----------|-------------------------|----------------|
|       | Decanoic acid (see capric acid)   |        |           |           |           |                         |                |
|       | Hexanoic acid (see caproic acid)  |        |           |           |           |                         |                |
|       | Mucic acid (see galactaric acid)  |        |           |           |           |                         |                |
|       | Octanoic acid (see caprylic acid) |        |           |           |           |                         |                |
| 1     | Hydrochloric acid                 | 36.46  | -6        | A         |           | n.s.                    | +              |
| 1     | Carbonic acid                     | 44.01  | 6.46      | A         | 10.3      | A                       | +              |
| 3     | Formic acid                       | 46.02  | 3.75      | A         |           |                         |                |
| 1     | Thiocyanic acid                   | 59.09  | -1.33     | A         |           |                         |                |
| 1     | Acetic acid                       | 60.05  | 4.756     | A         |           | n.s.                    | +              |
| 3     | Nitric Acid                       | 63.02  | -1.32     | A         |           |                         |                |
| 2     | Propionic acid                    | 74.08  | 4.87      | A         |           | n.s.                    | +              |
| 1     | Glycolic acid                     | 76.05  | 3.28      | A         |           |                         |                |
| 3     | Hydrobromic acid                  | 80.92  | < -6      | A         |           |                         |                |
| 2     | Isobutyric acid                   | 88.11  | 4.86      | A         |           |                         |                |
| 2     | Oxalic acid                       | 90.04  | 1.271     | A         | 4.266     | A                       |                |
| 1     | DL-Lactic acid                    | 90.08  | 3.86      | A         |           |                         | +              |
| 2     | Methanesulfonic acid              | 96.10  | -1.2      | A         |           |                         |                |
| 1     | Phosphoric acid                   | 98.00  | 1.96      | A         | 7.12      | A                       | 12.32          |
| 1     | Sulfuric acid                     | 98.08  | -3        | A         | 1.92      | A                       | n.s.           |
| 2     | Malonic acid                      | 104.06 | 2.826     | A         | 5.696     | A                       |                |
| 2     | Ethanesulfonic acid               | 110.13 | 2.05      | A         |           |                         |                |
| 1     | Fumaric acid                      | 116.08 | 3.03      | A         | 4.38      | A                       | 6              |
| 1     | Maleic acid                       | 116.08 | 1.92      | A         | 6.23      | A                       |                |
| 3     | Caproic acid (hexanoic acid)      | 116.16 | 4.8       | A         |           |                         |                |
| 1     | Succinic acid                     | 118.09 | 4.207     | A         | 5.635     | A                       | n.s.           |
| 2     | Benzoic acid                      | 122.12 | 4.19      | A         |           |                         | +              |
| 2     | Nicotinic acid                    | 123.11 | 4.85      | A         | 2.07      | B                       | +              |
| 2     | Ethanesulfonic acid, 2-hydroxy-   | 126.13 | 1.66      | A         |           |                         |                |
| 3     | Acetic acid, 2,2-dichloro-        | 128.95 | 1.35      | A         |           |                         |                |
| 2     | (-)-L-Pyroglutamic acid           | 129.11 | 3.32      | A         |           |                         |                |
| 1     | Glutaric acid                     | 132.12 | 4.34      | A         | 5.27      | A                       |                |
| 1     | L-Aspartic acid                   | 133.11 | 1.88      | A         | 3.65      | A                       | 9.60           |
| 1     | (-)-L-Malic acid                  | 134.09 | 3.459     | A         | 5.097     | A                       | n.s.           |
| 3     | Salicylic acid                    | 138.12 | 2.97      | A         | 13.82     | A                       |                |
| 2     | Caprylic acid (octanoic acid)     | 144.22 | 4.91      | A         |           |                         | n.s.           |
| 2     | Glutaric acid, 2-oxo-             | 146.10 | 2.7       | A         | 4.5       | A                       |                |
| 1     | Adipic acid                       | 146.14 | 4.44      | A         | 5.44      | A                       | 5              |

Table 3 (cont.)

| Class | Acid                                      | $M_r$   | $pK_{a1}$ | $pK_{a2}$ | $pK_{a3}$ | ADI<br>up to<br>[mg/kg] | GRAS<br>Status |
|-------|---|---------|-----------|-----------|-----------|-------------------------|----------------|
| 1     | Glutamic acid                             | 147.13  | 2.19      | A         | 4.25      | A                       | 9.67           |
| 3     | Cinnamic acid                             | 148.16  | 4.404     | A         |           |                         |                |
| 1     | (+)-L-Tartaric acid                       | 150.09  | 3.02      | A         | 4.36      | A                       |                |
| 3     | DL-Mandelic acid                          | 152.15  | 3.372     | A         |           |                         | +              |
| 3     | Salicylic acid, 4-amino-                  | 153.14  | 3.25      | A         | 10        | A                       | 3.5            |
| 2     | Gentisic acid                             | 154.12  | 2.93      | A         |           |                         |                |
| 2     | Orotic acid                               | 156.10  | 5.85      | A         | 8.95      | A                       |                |
| 2     | Benzenesulfonic acid                      | 158.18  | 0.7       | A         |           |                         |                |
| 1     | Glycerophosphoric acid                    | 172.08  | 1.47      | A         | 6.19      | A                       |                |
| 2     | <i>p</i> -Toluenesulfonic acid            | 172.21  | -1.34     | A         |           |                         |                |
| 1     | Capric acid (decanoic acid)               | 172.27  | 4.9       | A         |           |                         | n.s.           |
| 1     | L-Ascorbic acid                           | 176.13  | 4.17      | A         | 11.57     | A                       | +              |
| 1     | Hippuric acid                             | 179.17  | 3.55      | A         |           |                         |                |
| 3     | Benzoic acid, 4-acetamido-                | 179.18  | 4.3       | A         |           |                         |                |
| 2     | Cyclamic acid                             | 179.24  | ~-2.01    | A         |           |                         |                |
| 3     | Undecylenic acid<br>(undec-10-enoic acid) | 184.27  | 4.9       | A         |           |                         |                |
| 2     | 2-Naphthoic acid, 1-hydroxy-              | 188.17  | 2.7       | A         | 13.5      | A                       |                |
| 2     | Ethane-1,2-disulfonic acid                | 190.20  | -2.1      | A         | -1.5      | A                       |                |
| 1     | Citric acid                               | 192.13  | 3.128     | A         | 4.761     | A                       | 6.396          |
| 1     | D-Glucuronic acid                         | 194.14  | 3.18      | A         |           |                         | n.s.           |
| 1     | D-Gluconic acid                           | 196.16  | 3.76      | A         |           |                         | 50             |
| 2     | (+)-Camphoric acid                        | 200.24  | 4.716     | A         | 5.83      | A                       |                |
| 1     | Lauric acid                               | 200.32  | 4.9       | A         |           |                         | n.s.           |
| 1     | Sebacic acid                              | 202.25  | 4.59      | A         | 5.59      | A                       |                |
| 2     | Naphthalene-2-sulfonic acid               | 208.24  | 0.17      | A         |           |                         |                |
| 1     | Galactaric acid                           | 210.14  | 3.08      | A         | 3.63      | A                       |                |
| 1     | D-Glucoheptonic acid                      | 226.18  | 3.3       | A         |           |                         |                |
| 3     | (+)-Camphor-10-sulfonic acid              | 232.29  | 2.17      | A         |           |                         |                |
| 1     | Palmitic acid                             | 256.42  | 4.9       | A         |           |                         | n.s.           |
| 2     | Dodecylsulfuric acid                      | 266.40  | -0.09     | A         |           |                         |                |
| 2     | Oleic acid                                | 282.45  | ca. 4     | A         |           |                         |                |
| 1     | Stearic acid                              | 284.49  | 4.9       | A         |           |                         | n.s.           |
| 2     | Naphthalene-1,5-disulfonic acid           | 332.26  | -3.37     | A         | -2.64     | A                       |                |
| 2     | Lactobionic acid                          | 358.30  | 3.2       | A         |           |                         |                |
| 2     | Pamoic acid (embonic acid)                | 388.38  | 2.51      | A         | 3.1       | A                       |                |
| 2     | Alginic acid                              | 240 000 | ≥ 2.4     | A         |           |                         | n.s.           |

Table 4. Acids: Sorted by Class

| Acid                                      | $M_r$   | $pK_{a1}$  | $pK_{a2}$ | $pK_{a3}$ | ADI<br>up to<br>[mg/kg] | GRAS<br>Status |      |
|---|---------|------------|-----------|-----------|-------------------------|----------------|------|
| Decanoic acid (see <i>capric acid</i> )   |         |            |           |           |                         |                |      |
| Hexanoic acid (see <i>caproic acid</i> )  |         |            |           |           |                         |                |      |
| Mucic acid (see <i>galactaric acid</i> )  |         |            |           |           |                         |                |      |
| Octanoic acid (see <i>caprylic acid</i> ) |         |            |           |           |                         |                |      |
| <b>Class 1</b>                            |         |            |           |           |                         |                |      |
| Acetic acid                               | 60.05   | 4.756      | A         |           | n.s.                    | +              |      |
| Adipic acid                               | 146.14  | 4.44       | A         | 5.44      | A                       | 5              | +    |
| L-Ascorbic acid                           | 176.13  | 4.17       | A         | 11.57     | A                       |                | +    |
| L-Aspartic acid                           | 133.11  | 1.88       | A         | 3.65      | A                       | 9.60           | B    |
| Capric acid (decanoic acid)               | 172.27  | 4.9        | A         |           |                         | n.s.           |      |
| Carbonic acid                             | 44.01   | 6.46       | A         | 10.3      | A                       | n.s.           | +    |
| Citric acid                               | 192.13  | 3.128      | A         | 4.761     | A                       | 6.396          | A    |
| Fumaric acid                              | 116.08  | 3.03       | A         | 4.38      | A                       | 6              |      |
| Galactaric acid                           | 210.14  | 3.08       | A         | 3.63      | A                       |                |      |
| D-Glucoheptonic acid                      | 226.18  | 3.3        | A         |           |                         |                |      |
| D-Gluconic acid                           | 196.16  | 3.76       | A         |           |                         | 50             | #    |
| D-Glucuronic acid                         | 194.14  | 3.18       | A         |           |                         |                |      |
| Glutamic acid                             | 147.13  | 2.19       | A         | 4.25      | A                       | 9.67           | B    |
| Glutaric acid                             | 132.12  | 4.34       | A         | 5.27      | A                       |                |      |
| Glycerophosphoric acid                    | 172.08  | 1.47       | A         | 6.19      | A                       |                |      |
| Glycolic acid                             | 76.05   | 3.28       | A         |           |                         |                |      |
| Hippuric acid                             | 179.17  | 3.55       | A         |           |                         |                |      |
| Hydrochloric acid                         | 36.46   | -6         | A         |           |                         | n.s.           | +    |
| DL-Lactic acid                            | 90.08   | 3.86       | A         |           |                         |                | +    |
| Lauric acid                               | 200.32  | 4.9        | A         |           |                         | n.s.           |      |
| Maleic acid                               | 116.08  | 1.92       | A         | 6.23      | A                       |                |      |
| (-)-L-Malic acid                          | 134.09  | 3.459      | A         | 5.097     | A                       |                | n.s. |
| Palmitic acid                             | 256.42  | 4.9        | A         |           |                         | n.s.           |      |
| Phosphoric acid                           | 98.00   | 1.96       | A         | 7.12      | A                       | 12.32          | A    |
| Sebacic acid                              | 202.25  | 4.59       | A         | 5.59      | A                       |                |      |
| Stearic acid                              | 284.49  | 4.9        | A         |           |                         | n.s.           | +    |
| Succinic acid                             | 118.09  | 4.207      | A         | 5.635     | A                       | n.s.           | +    |
| Sulfuric acid                             | 98.08   | -3         | A         | 1.92      | A                       | n.s.           | +    |
| (+)-L-Tartaric acid                       | 150.09  | 3.02       | A         | 4.36      | A                       |                | +    |
| Thiocyanic acid                           | 59.09   | -1.33      | A         |           |                         |                |      |
| <b>Class 2</b>                            |         |            |           |           |                         |                |      |
| Alginate acid                             | 240 000 | $\geq 2.4$ | A         |           |                         | n.s.           | +    |
| Benzenesulfonic acid                      | 158.18  | 0.7        | A         |           |                         |                |      |
| Benzoic acid                              | 122.12  | 4.19       | A         |           |                         |                | +    |

Table 4 (cont.)

| Acid                                      | $M_r$  | $pK_{a1}$    | $pK_{a2}$ | $pK_{a3}$ | ADI<br>up to<br>[mg/kg] | GRAS<br>Status |
|---|--------|--------------|-----------|-----------|-------------------------|----------------|
| (+)-Camphoric acid                        | 200.24 | 4.716        | A         | 5.83      | A                       |                |
| Caprylic acid (octanoic acid)             | 144.22 | 4.91         | A         |           |                         | n.s.           |
| Cyclamic acid                             | 179.24 | $\sim -2.01$ | A         |           |                         |                |
| Dodecylsulfuric acid                      | 266.40 | $-0.09$      | A         |           |                         |                |
| Ethane-1,2-disulfonic acid                | 190.20 | $-2.1$       | A         | $-1.5$    | A                       |                |
| Ethanesulfonic acid                       | 110.13 | 2.05         | A         |           |                         |                |
| Ethanesulfonic acid, 2-hydroxy-           | 126.13 | 1.66         | A         |           |                         |                |
| Gentisic acid                             | 154.12 | 2.93         | A         |           |                         |                |
| Glutaric acid, 2-oxo-                     | 146.10 | 2.7          | A         | 4.5       | A                       |                |
| Isobutyric acid                           | 88.11  | 4.86         | A         |           |                         |                |
| Lactobionic acid                          | 358.30 | 3.2          | A         |           |                         |                |
| Malonic acid                              | 104.06 | 2.826        | A         | 5.696     | A                       |                |
| Methanesulfonic acid                      | 96.10  | $-1.2$       | A         |           |                         |                |
| Naphthalene-1,5-disulfonic acid           | 332.26 | $-3.37$      | A         | $-2.64$   | A                       |                |
| Naphthalene-2-sulfonic acid               | 208.24 | 0.17         | A         |           |                         |                |
| 2-Naphthoic acid, 1-hydroxy-              | 188.17 | 2.7          | A         | 13.5      | A                       |                |
| Nicotinic acid                            | 123.11 | 4.85         | A         | 2.07      | B                       |                |
| Oleic acid                                | 282.45 | ca. 4        | A         |           |                         | +              |
| Orotic acid                               | 156.10 | 5.85         | A         | 8.95      | A                       |                |
| Oxalic acid                               | 90.04  | 1.271        | A         | 4.266     | A                       |                |
| Pamoic acid (embonic acid)                | 388.38 | 2.51         | A         | 3.1       | A                       |                |
| Propionic acid                            | 74.08  | 4.87         | A         |           |                         | n.s.           |
| (-)-L-Pyroglutamic acid                   | 129.11 | 3.32         | A         |           |                         |                |
| p-Toluenesulfonic acid                    | 172.21 | $-1.34$      | A         |           |                         |                |
| <b>Class 3</b>                            |        |              |           |           |                         |                |
| Acetic acid, 2,2-dichloro-                | 128.95 | 1.35         | A         |           |                         |                |
| Benzoic acid, 4-acetamido-                | 179.18 | 4.3          | A         |           |                         |                |
| (+)-Camphor-10-sulfonic acid              | 232.29 | 2.17         | A         |           |                         |                |
| Caproic acid (hexanoic acid)              | 116.16 | 4.8          | A         |           |                         |                |
| Cinnamic acid                             | 148.16 | 4.404        | A         |           |                         |                |
| Formic acid                               | 46.02  | 3.75         | A         |           |                         |                |
| Hydrobromic acid                          | 80.92  | $< -6$       | A         |           |                         |                |
| DL-Mandelic acid                          | 152.15 | 3.372        | A         |           |                         |                |
| Nitric Acid                               | 63.02  | $-1.32$      | A         |           |                         |                |
| Salicylic acid                            | 138.12 | 2.97         | A         | 13.82     | A                       |                |
| Salicylic acid, 4-amino-                  | 153.14 | 3.25         | A         | 10        | A                       | 3.5            |
| Undecylenic acid<br>(undec-10-enoic acid) | 184.27 | 4.9          | A         |           |                         |                |

Table 5. Bases: Alphabetical Order

| Class | Base  | $M_r$  | $pK_{a1}$ | $pK_{a2}$ | $pK_{a3}$ | ADI<br>up to<br>[mg/kg] | GRAS<br>Status |
|-------|---|--------|-----------|-----------|-----------|-------------------------|----------------|
| 1     | Ammonia   | 17.03  | 9.27      | B         |           |                         | #              |
| 1     | L-Arginine  | 174.20 | 13.2      | B         | 9.09      | B 2.18                  | A              |
| 2     | Benethamine                                       | 197.28 | 4.46      | B         |           |                         |                |
| 2     | Benzathine  | 240.35 | 9.99      | B         | 9.39      | B                       |                |
| 2     | Betaine   | 117.15 | 12.16     | B         |           |                         |                |
| 1     | Calcium hydroxide                                 | 74.10  | 12.6      | B         | 11.57     | B                       | +              |
| 1     | Choline   | 121.18 | > 11      | B         |           |                         | #              |
| 2     | Deanol  | 89.14  | 8.83      | B         |           |                         |                |
| 3     | Diethanolamine<br>(2,2'-iminobis(ethanol))        | 105.14 | 9.28      | B         |           |                         |                |
| 2     | Diethylamine                                      | 73.14  | 10.93     | B         |           |                         |                |
| 2     | Ethanol, 2-(diethylamino)-                        | 117.19 | 9.58      | B         |           |                         |                |
| 3     | Ethanolamine (2-aminoethanol)                     | 61.08  | 9.50      | B         |           |                         |                |
| 3     | Ethylenediamine                                   | 60.10  | 7.00      | B         | 10.09     | B                       |                |
| 1     | Glucamine, <i>N</i> -methyl-                      | 195.22 | 8.03      | B         |           |                         |                |
| 2     | Hydrabamine                                       | 596.99 | 11.92     | B         | 11.32     | B                       |                |
| 3     | 1 <i>H</i> -Imidazole                             | 68.08  | 7.03      | B         |           |                         |                |
| 1     | Lysine  | 146.19 | 10.79     | B         | 9.18      | B 2.16                  | A              |
| 1     | Magnesium hydroxide                               | 58.33  | 11.4      | B         |           |                         | +              |
| 2     | Morpholine, 4-(2-hydroxyethyl)-                   | 131.18 | 7.39      | B         |           |                         |                |
| 3     | Piperazine  | 86.14  | 5.68      | B         | 9.82      | B                       |                |
| 1     | Potassium hydroxide                               | 56.11  | ca. 14    | B         |           |                         | +              |
| 2     | Pyrrolidine, 1-(2-hydroxyethyl)-                  | 115.18 | 9.44      | B         |           |                         |                |
| 1     | Sodium hydroxide                                  | 40.00  | ca. 14    | B         |           |                         | +              |
| 3     | Triethanolamine<br>(2,2',2"-nitrilotris(ethanol)) | 149.19 | 7.82      | B         |           |                         |                |
| 2     | Tromethamine                                      | 121.14 | 8.02      | B         |           |                         |                |
| 3     | Zinc hydroxide                                    | 99.38  | ca. 14    | B         | 9.64      | B                       | #              |

Table 6. Bases: Sorted by Decreasing  $pK_a$  Value

| Class | Base  | $M_r$  | $pK_{a1}$ | $pK_{a2}$ | $pK_{a3}$ | ADI<br>up to<br>[mg/kg] | GRAS<br>Status |
|-------|---|--------|-----------|-----------|-----------|-------------------------|----------------|
| 1     | Potassium hydroxide                               | 56.11  | ca. 14    | B         |           |                         | +              |
| 1     | Sodium hydroxide                                  | 40.00  | ca. 14    | B         |           |                         | +              |
| 3     | Zinc hydroxide                                    | 99.38  | ca. 14    | B         | 9.64      | B                       | #              |
| 1     | L-Arginine  | 174.20 | 13.2      | B         | 9.09      | B 2.18                  | A              |
| 1     | Calcium hydroxide                                 | 74.10  | 12.6      | B         | 11.57     | B                       | +              |
| 2     | Betaine   | 117.15 | 12.16     | B         |           |                         |                |
| 2     | Hydrabamine                                       | 596.99 | 11.92     | B         | 11.32     | B                       |                |
| 1     | Magnesium hydroxide                               | 58.33  | 11.4      | B         |           |                         | +              |
| 1     | Choline   | 121.18 | > 11      | B         |           |                         | #              |
| 2     | Diethylamine                                      | 73.14  | 10.93     | B         |           |                         |                |
| 1     | Lysine  | 146.19 | 10.79     | B         | 9.18      | B 2.16                  | A              |
| 2     | Benzathine  | 240.35 | 9.99      | B         | 9.39      | B                       |                |
| 2     | Ethanol, 2-(diethylamino)-                        | 117.19 | 9.58      | B         |           |                         |                |
| 3     | Ethanolamine (2-aminoethanol)                     | 61.08  | 9.50      | B         |           |                         |                |
| 2     | Pyrrolidine, 1-(2-hydroxyethyl)-                  | 115.18 | 9.44      | B         |           |                         |                |
| 3     | Diethanolamine<br>(2,2'-iminobis(ethanol))        | 105.14 | 9.28      | B         |           |                         |                |
| 1     | Ammonia   | 17.03  | 9.27      | B         |           |                         | #              |
| 2     | Deanol  | 89.14  | 8.83      | B         |           |                         |                |
| 1     | Glucamine, <i>N</i> -methyl-                      | 195.22 | 8.03      | B         |           |                         |                |
| 2     | Tromethamine                                      | 121.14 | 8.02      | B         |           |                         |                |
| 3     | Triethanolamine<br>(2,2',2"-nitrilotris(ethanol)) | 149.19 | 7.82      | B         |           |                         |                |
| 2     | Morpholine, 4-(2-hydroxyethyl)-                   | 131.18 | 7.39      | B         |           |                         |                |
| 3     | 1 <i>H</i> -Imidazole                             | 68.08  | 7.03      | B         |           |                         |                |
| 3     | Ethylenediamine                                   | 60.10  | 7.00      | B         | 10.09     | B                       |                |
| 3     | Piperazine  | 86.14  | 5.68      | B         | 9.82      | B                       |                |
| 2     | Benethamine                                       | 197.28 | 4.46      | B         |           |                         |                |

Table 7. Bases: Sorted by Increasing Molecular Weight

| Class | Base   | $M_r$  | $pK_{a1}$ | $pK_{a2}$ | $pK_{a3}$ | ADI<br>up to<br>[mg/kg] | GRAS<br>Status |
|-------|--|--------|-----------|-----------|-----------|-------------------------|----------------|
| 1     | Ammonia  | 17.03  | 9.27      | B         |           |                         | #              |
| 1     | Sodium hydroxide                                   | 40.00  | ca. 14    | B         |           |                         | +              |
| 1     | Potassium hydroxide                                | 56.11  | ca. 14    | B         |           |                         | +              |
| 1     | Magnesium hydroxide                                | 58.33  | 11.4      | B         |           |                         | +              |
| 3     | Ethylenediamine                                    | 60.10  | 7.00      | B         | 10.09     | B                       |                |
| 3     | Ethanolamine (2-aminoethanol)                      | 61.08  | 9.50      | B         |           |                         |                |
| 3     | 1 <i>H</i> -Imidazole                              | 68.08  | 7.03      | B         |           |                         |                |
| 2     | Diethylamine                                       | 73.14  | 10.93     | B         |           |                         |                |
| 1     | Calcium hydroxide                                  | 74.10  | 12.6      | B         | 11.57     | B                       | +              |
| 3     | Piperazine   | 86.14  | 5.68      | B         | 9.82      | B                       |                |
| 2     | Deanol   | 89.14  | 8.83      | B         |           |                         |                |
| 3     | Zinc hydroxide                                     | 99.38  | ca. 14    | B         | 9.64      | B                       | #              |
| 3     | Diethanolamine<br>(2,2'-iminobis(ethanol))         | 105.14 | 9.28      | B         |           |                         |                |
| 2     | Pyrrolidine, 1-(2-hydroxyethyl)-                   | 115.18 | 9.44      | B         |           |                         |                |
| 2     | Betaine  | 117.15 | 12.16     | B         |           |                         |                |
| 2     | Ethanol, 2-(diethylamino)-                         | 117.19 | 9.58      | B         |           |                         |                |
| 2     | Tromethamine                                       | 121.14 | 8.02      | B         |           |                         |                |
| 1     | Choline  | 121.18 | > 11      | B         |           |                         | #              |
| 2     | Morpholine, 4-(2-hydroxyethyl)-                    | 131.18 | 7.39      | B         |           |                         |                |
| 1     | Lysine   | 146.19 | 10.79     | B         | 9.18      | B 2.16                  | A              |
| 3     | Triethanolamine<br>(2,2',2''-nitrilotris(ethanol)) | 149.19 | 7.82      | B         |           |                         |                |
| 1     | L-Arginine   | 174.20 | 13.2      | B         | 9.09      | B 2.18                  | A              |
| 1     | Glucamine, <i>N</i> -methyl-                       | 195.22 | 8.03      | B         |           |                         |                |
| 2     | Benethamine  | 197.28 | 4.46      | B         |           |                         |                |
| 2     | Benzathine   | 240.35 | 9.99      | B         | 9.39      | B                       |                |
| 2     | Hydrabamine  | 596.99 | 11.92     | B         | 11.32     | B                       |                |

Table 8. Bases: Sorted by Class

| Base   | $M_r$  | $pK_{a1}$ | $pK_{a2}$ | $pK_{a3}$ | ADI<br>up to<br>[mg/kg] | GRAS<br>Status |
|--|--------|-----------|-----------|-----------|-------------------------|----------------|
| <b>Class 1</b>                                     |        |           |           |           |                         |                |
| Ammonia  | 17.03  | 9.27      | B         |           |                         | #              |
| L-Arginine   | 174.20 | 13.2      | B         | 9.09      | B 2.18                  | A              |
| Calcium hydroxide                                  | 74.10  | 12.6      | B         | 11.57     | B                       | +              |
| Choline  | 121.18 | > 11      | B         |           |                         | #              |
| Glucamine, <i>N</i> -methyl-                       | 195.22 | 8.03      | B         |           |                         |                |
| Lysine   | 146.19 | 10.79     | B         | 9.18      | B 2.16                  | A              |
| Magnesium hydroxide                                | 58.33  | 11.4      | B         |           |                         | +              |
| Potassium hydroxide                                | 56.11  | ca. 14    | B         |           |                         | +              |
| Sodium hydroxide                                   | 40.00  | ca. 14    | B         |           |                         | +              |
| <b>Class 2</b>                                     |        |           |           |           |                         |                |
| Benethamine  | 197.28 | 4.46      | B         |           |                         |                |
| Benzathine   | 240.35 | 9.99      | B         | 9.39      | B                       |                |
| Betaine  | 117.15 | 12.16     | B         |           |                         |                |
| Deanol   | 89.14  | 8.83      | B         |           |                         |                |
| Diethylamine                                       | 73.14  | 10.93     | B         |           |                         |                |
| Ethanol, 2-(diethylamino)-                         | 117.19 | 9.58      | B         |           |                         |                |
| Hydrabamine  | 596.99 | 11.92     | B         | 11.32     | B                       |                |
| Morpholine, 4-(2-hydroxyethyl)-                    | 131.18 | 7.39      | B         |           |                         |                |
| Pyrrolidine, 1-(2-hydroxyethyl)-                   | 115.18 | 9.44      | B         |           |                         |                |
| Tromethamine                                       | 121.14 | 8.02      | B         |           |                         |                |
| <b>Class 3</b>                                     |        |           |           |           |                         |                |
| Diethanolamine<br>(2,2'-iminobis(ethanol))         | 105.14 | 9.28      | B         |           |                         |                |
| Ethanolamine (2-aminoethanol)                      | 61.08  | 9.50      | B         |           |                         |                |
| Ethylenediamine                                    | 60.10  | 7.00      | B         | 10.09     | B                       |                |
| 1 <i>H</i> -Imidazole                              | 68.08  | 7.03      | B         |           |                         |                |
| Piperazine   | 86.14  | 5.68      | B         | 9.82      | B                       |                |
| Triethanolamine<br>(2,2',2''-nitrilotris(ethanol)) | 149.19 | 7.82      | B         |           |                         |                |
| Zinc hydroxide                                     | 99.38  | ca. 14    | B         | 9.64      | B                       | #              |