**APPENDIX I**

Substituent constants used in LFER equations

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| S.No. | Substittuents  X | σp | σpo | σp+ |
|  |  |  |  |  |
| 1. | -NMe2 | -0.83 |  | -1.7 |
|  |  |  |  |  |
| 2. | -OCH3 | -0.27 | -0.12 | -0.78 |
|  |  |  |  |  |
| 3. | -OH | -0.37 |  | -0.92 |
|  |  |  |  |  |
| 4. | -CH3 | -0.17 | -0.14 | -0.31 |
|  |  |  |  |  |
| 5. | -H | 0 | 0 | 0 |
|  |  |  |  |  |
| 6. | -Cl | 0.23 | 0.34 | 0.11 |
|  |  |  |  |  |
| 7. | -Br | 0.23 | 0.22 | 0.15 |
|  |  |  |  |  |
| 8. | -CHO | 0.42 |  | 0.73 |
|  |  |  |  |  |
| 9. | -COOH | 0.45 | 0.44 | 0.42 |
|  |  |  |  |  |
| 10. | -NO2 | 0.75 | 0.81 | 0.79 |
|  |  |  |  |  |

Substituent constants used for dual-parameter correaltions

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| S.No. | Substituents  X | σI | σR | σRo | σR+ | σR- | F | R | ν |
|  |  |  |  |  |  |  |  |  |  |
| 1. | -NMe2 | 0.1 | -0.83 |  | -1.7 | -0.34 |  |  |  |
|  |  |  |  |  |  |  |  |  |  |
| 2. | -OCH3 | 0.26 | -0.61 | -0.41 | -1.02 | -0.45 | 0.29 | -0.56 | 0.36 |
|  |  |  |  |  |  |  |  |  |  |
| 3. | -OH | 0.27 | -0.43 |  | -0.44 |  | 0.33 | -0.7 | 0.32 |
|  |  |  |  |  |  |  |  |  |  |
| 4. | -CH3 | -0.05 | -0.11 | -0.1 | -1.25 | -0.11 | 0.01 | -0.18 | 0.52 |
|  |  |  |  |  |  |  |  |  |  |
| 5. | -H | 0 | 0 | 0 | 0 | 0 | 0.03 | 0 | 0 |
|  |  |  |  |  |  |  |  |  |  |
| 6. | -Cl | 0.47 | -0.23 | -0.21 | -0.23 | -0.35 | 0.42 | -0.19 | 0.55 |
|  |  |  |  |  |  |  |  |  |  |
| 7. | -Br | 0.45 | -0.19 | -0.61 | -0.19 | -0.3 | 0.45 | -0.22 | 0.65 |
|  |  |  |  |  |  |  |  |  |  |
| 8. | -COOH | 0.3 | -0.08 |  | 0.43 | 0.06 |  |  |  |
|  |  |  |  |  |  |  |  |  |  |
| 9. | -NO2 | 0.64 | 0.15 | 0.19 | 0.15 | 0.46 | 0.65 | 0.13 | 1.39 |
|  |  |  |  |  |  |  |  |  |  |