|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| S.No. | Substituents  X | σp | σpo | σp+ |
|  |  |  |  |  |
| 1. | -OCH3 | -0.27 | -0.12 | -0.78 |
|  |  |  |  |  |
| 2. | -CH3 | -0.17 | -0.14 | -0.31 |
|  |  |  |  |  |
| 3. | -Cl | 0.23 | 0.34 | 0.11 |
|  |  |  |  |  |
| 4. | -H | 0 | 0 | 0 |
|  |  |  |  |  |
| 5. | -Br | 0.23 | 0.22 | 0.15 |
|  |  |  |  |  |
| 6. | -COOH | 0.45 | 0.44 | 0.42 |
|  |  |  |  |  |

Appendix I

Substituent constants used for LFER calculations

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| S.No. | Substituents  X | σI | σR | σR+ | σR- | F | R |
|  |  |  |  |  |  |  |  |
|  | -OCH3 | 0.26 | -0.61 | -1.02 | -0.45 | 0.29 | -0.56 |
|  |  |  |  |  |  |  |  |
|  | -CH3 | -0.05 | -0.11 | -1.25 | -0.11 | 0.01 | -0.18 |
|  |  |  |  |  |  |  |  |
|  | -Cl | 0.47 | -0.23 | -0.23 | -0.35 | 0.42 | -0.19 |
|  |  |  |  |  |  |  |  |
|  | -H | 0 | 0 | 0 | 0 | 0.03 | 0 |
|  |  |  |  |  |  |  |  |
|  | -Br | 0.45 | -0.19 | -0.19 | -0.3 | 0.45 | -0.22 |
|  |  |  |  |  |  |  |  |
|  | -COOH | 0.3 | -0.08 | 0.43 | 0.06 |  |  |
|  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |