Table I. Global reactivity descriptors evaluated for TB and its dechlorinated forms at the wB97XD/6-311++G(2d,2p) level of theory in the aqueous phase, employing the PCM solvation model, according to the equations (1), (3) and (4).

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **  /eV | **  /eV | **  /eV |  | **  /eV | **  /eV | **  /eV |
| TB | 0.22 | -0.15 | 0.05 | DTB | 0.22 | -0.14 | 0.04 |
| TBS | 0.22 | -0.15 | 0.05 | DTBS | 0.22 | -0.15 | 0.05 |
| TBSu | 0.22 | -0.15 | 0.05 | DTBSu | 0.24 | -0.15 | 0.05 |