| $_{\omega}$ B2PLYP'/def2-SV(P) (adiabatic) | | | | |
|--|--|--|--|--------------------------|
| Molecule | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$ | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $f_{12}(S_0\text{-}S_1)$ |
| S1703 | 1.8465 | 1.8120 | 0.0345 | - |
| S1704 | 1.9536 | 1.8921 | 0.0615 | - |
| S1705 | 1.9284 | 1.8892 | 0.0392 | - |
| S1706 | 2.0287 | 1.9545 | 0.0742 | - |
| S1707 | 2.1660 | 2.0712 | 0.0948 | - |
| S1708 | 2.2840 | 2.1548 | 0.1292 | - |
| S1709 | 2.2467 | 2.1603 | 0.0865 | - |
| S1710 | 2.3598 | 2.2190 | 0.1409 | - |
| S1711 | 2.4501 | 2.4554 | -0.0053 | - |
| S635 | 2.5757 | 2.5107 | 0.0649 | - |
| S1712 | 2.5485 | 2.5048 | 0.0437 | - |
| S1713 | 2.7165 | 2.5367 | 0.1798 | - |
| S559 | 2.4270 | 2.3821 | 0.0450 | - |
| S1714 | 2.5100 | 2.4535 | 0.0565 | - |
| S1715 | 2.5139 | 2.4927 | 0.0212 | - |
| S1716 | 2.5821 | 2.5413 | 0.0408 | - |