|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | vdW  [kcal mol−1] | ES  [kcal mol−1] | polar  [kcal mol−1] | non-polar  [kcal mol−1] | total  [kcal mol−1] |
| WT | −28.19 ± 0.08 | −46.96 ± 0.08 | 43.51 ± 0.06 | −3.54 ± 0.00 | −35.19 ± 0.07 |
| H274Y | −22.50 ± 0.09 | −40.82 ± 0.10 | 39.35 ± 0.08 | −3.31 ± 0.00 | −27.28 ± 0.09 |