

Decane

| | | | | | | | | |
|-------------------|---------------|----------------------------|---------------|---------------|---------------|---------------|---------------|---------------|
| C10H22 | | | | | | | | |
| pi | nu 0 | e | h bar | m sub e | a0 | c | mp | |
| | 3.1415927E+00 | 1.2566371E-06 | 1.6021892E-19 | 1.0545888E-34 | 9.1095345E-31 | 5.2917706E-11 | 2.9979246E+08 | 1.6726486E-27 |
| | epsilon 0 | uB | eV/cm^-1 | | aH | | md | |
| | | 8.85E-12 | 9.27E-24 | 0.000123985 | 5.29465E-11 | | | 3.3435860E-27 |
| cm-1/eV | | | | | | | | |
| | 1.239810E-04 | | | | | | | |
| kcal/mole/eV | | Total Bond Energy CH3 (eV) | | | | | | |
| | | 12.49186 | | | | | | |
| | 4.336340E-02 | | | | | | | |
| kJ/mole/eV | | Total Bond Energy CH2 (eV) | | | | | | |
| | | 7.83016 | | | | | | |
| | 0.010364101 | | | | | | | |
| C | | Total Bond Energy C-C (eV) | | | | | | |
| | | 4.32754 | | | | | | |
| | 716.68 | | | | | | | |
| | 7.42774 | | | | | | | |
| H | | Decane Total E (eV) | | | | | | |
| | | 126.57286 | | | | | | |
| | 217.998 | | | | | | | |
| | 2.259353 | | | | | | | |
| decane | | Exp Decane Total E (eV) | | | | | | |
| | | 126.56906 | | | | | | |
| | -249.5 | | | | | | | |
| | -2.5858 | | | | | | | |
| | | Rel. Error | | | | | | |
| | | -3.0033E-05 | | | | | | |
| | 123.9832155 | | | | | | | |
| total bond energy | | | | | | | | |
| | 126.56906 | | | | | | | |