

Octane

C8H18							
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		Octane Total E (eV)					
		102.25746					
	217.998						
	2.259353						
octane		Exp Octane Total E (eV)					
		102.25123					
	-208.5						
	-2.1609						
		Rel. Error					
		-6.09396E-05					
	100.0903137						
total bond energy							
	102.25123						