(a) $\Delta\Delta H^\circ_{\mathrm{f},298}$ (kcal/mol)

(b) ΔS°_{298} (cal/mol/K)

(c) $\Delta C_{\mathrm{p},300}$ (cal/mol/K)

(d) $\Delta C_{\mathrm{p},400}$ (cal/mol/K)

(e) $\Delta C_{\mathrm{p},500}$ (cal/mol/K)

(f) $\Delta C_{\mathrm{p},600}$ (cal/mol/K)

(g) $\Delta C_{\mathrm{p},800}$ (cal/mol/K)

(h) $\Delta C_{\mathrm{p},1000}$ (cal/mol/K)

(i) $\Delta C_{\mathrm{p},1500}$ (cal/mol/K)

Unc. est. / $\sqrt{\text{test error}^2 + \text{data unc.}^2}$ (N=274)

| Test error |

Empirical

SIDT

Finetuned empirical