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COMPUTED HEATS OF FORMATION

by

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Computed heats of formation for 1 - 4.

1: $\Delta H_f^{298K}$ (solid) = 157 kcal/mole = 524 cal/g
2: $\Delta H_f^{298K}$ (solid) = 46 kcal/mole = 183 cal/g
3: $\Delta H_f^{298K}$ (solid) = 59 kcal/mole = 250 cal/g
4: $\Delta H_f^{298K}$ (solid) = 143 kcal/mole = 918 cal/g

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13. ABSTRACT (Maximum 200 words)
Computed heats of formation for 1 - 4.

energetic compounds; heats of formation
We have used our density functional procedure [1] to compute the heats of formation of the compounds 1 - 4, in response to a request from R. Naylor (Allegheny Ballistics Laboratory). The vibrational energies were determined from the molecular stoichiometries [2]. The density functional calculations give the gas phase heat of formation, which we convert to the liquid and solid state values by subtracting, respectively, the heat of vaporization and the heat of sublimation. These are obtained by means of relationships that we have developed involving the computed electrostatic potential on the molecular surface [3,4].

**Results:**

1.

\[
\Delta H_f^{298K} \text{(gas)} = 189 \text{ kcal/mole} = 630 \text{ cal/g} \\
\Delta H_f^{298K} \text{(liquid)} = 174 \text{ kcal/mole} = 579 \text{ cal/g} \\
\Delta H_f^{298K} \text{(solid)} = 157 \text{ kcal/mole} = 524 \text{ cal/g}
\]

2.

\[
\Delta H_f^{298K} \text{(gas)} = 76 \text{ kcal/mole} = 304 \text{ cal/g} \\
\Delta H_f^{298K} \text{(liquid)} = 60 \text{ kcal/mole} = 243 \text{ cal/g} \\
\Delta H_f^{298K} \text{(solid)} = 46 \text{ kcal/mole} = 183 \text{ cal/g}
\]

3.

\[
\Delta H_f^{298K} \text{(gas)} = 85 \text{ kcal/mole} = 364 \text{ cal/g} \\
\Delta H_f^{298K} \text{(liquid)} = 71 \text{ kcal/mole} = 303 \text{ cal/g} \\
\Delta H_f^{298K} \text{(solid)} = 59 \text{ kcal/mole} = 250 \text{ cal/g}
\]

4.

\[
\Delta H_f^{298K} \text{(gas)} = 165 \text{ kcal/mole} = 1058 \text{ cal/g} \\
\Delta H_f^{298K} \text{(liquid)} = 152 \text{ kcal/mole} = 974 \text{ cal/g} \\
\Delta H_f^{298K} \text{(solid)} = 143 \text{ kcal/mole} = 918 \text{ cal/g}
\]

For comparison, the experimental gas phase \( \Delta H_f^{298K} \) value for RDX is 206 cal/g [5,6].
References: