The predicted heat of formation and impact sensitivity of the recently-synthesized dinitro-N-fluorotriazole 1,

\[
\begin{align*}
\text{NO}_2 & \\
\text{N} & \\
\text{N} & \\
\text{O}_2\text{N} & \\
\text{N} & \\
\text{F} &
\end{align*}
\]

based on computational analyses, are:

\[
\Delta H_f (\text{gaseous}) = 77 \text{ kcal/mole} = 435 \text{ cal/gram} \\
\Delta H_f (\text{solid}) = 56 \text{ kcal/mole} = 316 \text{ cal/gram} \\
h_{50} = 126 \text{ cm}
\]
COMPULATED HEAT OF FORMATION AND IMPACT SENSITIVITY
OF A NEW DINITRO-N-FLUOROTRIAZOLE

by

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The dinitro-N-fluorotriazole 1 has recently been synthesized [1] and characterized crystallographically [2].

![Chemical Structure](attachment:1.png)

We now report our computed heat of formation and impact sensitivity for 1.

The gas phase heat of formation was calculated using our density functional procedure [3]. It was converted to the solid phase value by means of eq. (1),

\[
\Delta H_f \text{ (solid)} = \Delta H_f \text{ (gaseous)} - \Delta H_{sub}
\]

(1)

in which \(\Delta H_{sub}\) is the heat of sublimation. \(\Delta H_{sub}\) and the impact sensitivity, \(h_{50}\), were obtained by means of correlations that we have developed between these properties and computed quantities related to electrostatic potentials on molecular surfaces [4,5]. The latter were calculated at the \textit{ab initio} HF/STO-5G//HF/3-21G level.

The results follow:

\[
\Delta H_f \text{ (gaseous)} = 77 \text{ kcal/mole} = 435 \text{ cal/gram}
\]

\[
\Delta H_f \text{ (solid)} = 56 \text{ kcal/mole} = 316 \text{ cal/gram}
\]

\(h_{50} = 126 \text{ cm}\)

References