NIST Chemistry WebBook

NIST Standard Reference Database Number 69

View: Search Options, Models and Tools, Special Data Collections, Documentation, Changes, Notes

Show Credits

NIST reserves the right to charge for access to this database in the future.

Search Options top

General Searches

Physical Property Based Searches

- Formula
- Name
- Ion energetics properties Vibrational and electronic energies Molecular weight
- IUPAC identifier
- CAS registry number
- Reaction
- Author Structure

Models and Tools top

- ical Properties of Fluid Systems: High accuracy data for a select group of fluids.
- Group Additivity Based Estimates: Estimates of gas phase thermodynamic properties based on a submitted structure.
 Formula Browser: Locates chemical species by building up a chemical formula in Hill order.

Special Data Collections top

- Benchmark Spray Combustion Database: A collection of spray combustion data from experiments conducted at NIST.
- Droplet Laden Flow Data: Results from experiments involving flow over cylinders.

Documentation top

- Frequently asked questions
- A Guide to the NIST Chemistry WebBook: A guide to this site and the data available from it.
- Gas-Phase Ion Thermochemistry: An in-depth explanation of gas phase ion data available from this site
- NIST Organic Thermochemistry Archive: A description of the primary source of thermochemical data for this site.

 Organometallic Thermochemistry Database: A description of the organometallic thermochemistry database included in this site.

 Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules: A description of vibrational and electronic energy level data for molecules with three or more atoms.

 Computed 3-D Structures: A description of the manner in which the 3 dimensional structures on this site were generated.
- Evaluated Infrared Spectra: A description of one of the collections of IR spectra available on this site. Quantitative Infrared Database: A description of the NIST Quantitative Infrared Database.
- THz Spectral Database: A description of THz infrared spectra measured by NIST.
- UV/Vis Database User's Guide: A description of the UV/Vis spectra available from this site.

 Gas Chromatographic Retention Data: A description of the retention index data available from this site.
- Citation Guide: A Guide to the proper citation of data from this site.
- Species List: A list of all of the chemical species in this release of the NIST Chemistry WebBook.

Recent changes to this site top

Last changes to the site: September 27, 2012

Recent changes:

- Added additional three dimensional structures.
- Added a Java based viewer for three dimensional structures
- Added droplet laden flow data
- Updated thermochemical data for gas phase ions and ion clusters.

Notes top

This site provides thermochemical, thermophysical, and ion energetics data compiled by NIST under the Standard Reference Data Program.

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