

The NIST Retention Index Database

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The NIST Retention Database is a collection of gas chromatographic retention indices compiled from the regular journal papers, review papers, Internet sources, and technical reports. Retention indices a normalized measure of the time required for a chemical species to traverse a chromatography column (retention time). The retention index of a substance is a physico-chemical property that has been correlated with boiling point and heat of vaporization.

The database includes Kovats and Lee retention indices for columns with non-polar phases. Work is currently underway to extend the database to columns with polar phases. At the present time the database contains over 120,000 retention index values corresponding to over 25,000 different chemical species. The database is available as part of the NIST/EPA/NIH Mass Spectral Database or for free on the web at the NIST Chemistry WebBook site (<http://webbook.nist.gov>). An important application of the database is to disambiguate GC-MS results for species with similar mass spectra, but differing retention indices.

In this presentation we will provide a concise overview of the database including discussion of the manner in which the database is developed and the steps taken to insure quality in the database. Data were entered using custom software and reviewed prior to the release of the database. This review procedure includes the use of statistical analyses of data and comparisons with structure-based models.