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Determination of the Lipophilicity Parameters R_{M0} and Log$P$ of New Azaphenothiazines by Reversed-Phase Thin-Layer Chromatography†

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Abstract

The lipophilicity parameters (R_{M0} and $logP_{TLC}$) of three types of azaphenothiazines 1–3 were determined by reversed-phase thin-layer chromatography on RP-18 silica plates with acetone-aqueous TRIS (tris(hydroxymethyl)aminomethane) buffer as the mobile phase. The R_M values were linearly dependent on the concentration of acetone, and extrapolated to 0% of acetone, gave the lipophilicity parameter R_{M0}. The parameter R_{M0} and specific hydrophobic surface area b were significantly intercorrelated showing a congeneric class of azaphenothiazines 1–3. The parameter $logP_{TLC}$ was determined from the R_{M0} values by use of a calibration curve obtained for five standards. The determined parameters were discussed in the terms of structure lipophilicity relationships and compared with data obtained from seven calculation programs.

Keywords:

Lipophilicity parameters | R_{M0} | LogP | Azaphenothiazines | Reversed-phase | TLC

Notes

[†]Part XCI in the series of Azinyl Sulfides.

Multivariate analysis of experimental and computational descriptors of molecular lipophilicity.

Source: Journal of Computer-Aided Molecular Design

UNEXPECTED SIMPLE ROUTE TO NOVEL DIPYRIDO-1,4-THIAZINE SYSTEM

Source: Heterocyclic Communications

Azinyl sulfides. L. 14-Methyl-1,4-thiazino[2,3-c;6,5-c′]diquinoline

Source: Acta Crystallographica Section C Crystal Structure Communications

Octanol: Water partition coefficients (P): Measurement, estimation, and interpretation, particularly for chemicals with P > 105

Source: Ecotoxicology and Environmental Safety

Azinyl sulfides. L.

Source: Acta Crystallographica Section C Crystal Structure Communications

A new method for the estimation of partition coefficient

Source: Journal of the American Chemical Society

Determination of lipophilicity by means of reversed-phase thin-layer chromatography

Source: Journal of Chromatography A

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