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Determination of the Lipophilicity Parameters R_{M0} and LogP of New Azaphenothiazines by Reversed-Phase Thin-Layer Chromatography[†]

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Abstract

The lipophilicity parameters (R_{M0} and $\log P_{TLC}$) 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 $\log P_{TLC}$ 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.

Lipophilicity parameters

R_{M0}

LogP

Azaphenothiazines

Reversed-phase

TLC

Notes

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

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[Calculation Procedures for Molecular Lipophilicity: a Comparative Study](#)

Source: Quantitative Structure-Activity Relationships

[Calculating log Poct from structures](#)

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[Lipophilicity of Some N- and O-Substituted Alkanoic Acids of 1,2-Benzisothiazol-3\(2H\)-one Determined by Reversed-Phase Thin Layer Chromatography](#)

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