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SCREENING RESULTS ON THE TOXICITY OF NUMEROUS FLUORO ORGANIC COMPOUNDS

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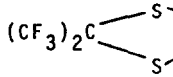
It is almost impossible to predict the toxicity of organic fluorine compounds on the basis of chemical structure related elements. As a matter of fact, closely related substances may possess strikingly different toxic properties. On the grounds of working safely with new chemicals, we were interested in setting up a quick and simple pre-screening test using NRMI-mice to get preliminary data on acute inhalation toxicities of volatile fluorine compounds. We now report on experimental procedure, evaluation and results of such tests and - a point of much importance - the correlation between the pre-screening data and those obtained from some more elaborate LC_{50} studies (4 h). We determined, besides others, the following pre-screening data (1 h) (in parentheses: values given in ppm), in addition to those published in J. Fluorine Chemistry, 21(1) (1982):

ICF_2CF_2I (50-100), $CF_3CF_2CF_2CI(CF_3)_2$ (< 50), CF_3-$CF(CF_3)$-CF_2-CFI-CF_3 (250-500), CF_3-CF_2-$C(CF_3)_2I$ (< 50), $(CF_3)_3CI$ (< 100), HCF_2-CF_2-$CFBr$-CF_2Br (< 100), $(CF_3)_2CBr$-CF_2-CF_2-CF_3 (< 100), C_6F_{13}-$CHCl$-CH_2Cl (> 5.000), C_6F_{13}-$CHBr$-CH_2Br (> 5.000), CF_3-$CFCl$-$CFCl$-$CF(CF_3)_2$ (500-1.000), CF_2Br-$CFCl$-CH_2-CH_2Br (1.000-2.500), $CF_3CF_2CH_2CH_2I$ (100-500), CF_2-CF_2-CH=CCl (100-500), $(CF_3)_2C$=$C(OCH_3)C_2F_5$ (1.000-2.500), CF_3-CF_2-CF=$C(CF_3)_2$ (100-250), C_4F_9-CBr=CH_2 (> 10.000), CH_2=$CH(CF_2)_4CH$=CH_2 (2.500-5.000), C_4F_9-CH=CF_2 (5.000-10.000), $(CF_3)_2C$=CH_2 (500-1.000), CH_2=CH-CH_2-O-$C(O)$-CF_2H (2.500-5.000), CH_2=CH-$C(O)$-O-CH_2-CF_2-CFH-CF_3 (2.500-5.000), CH_2=$C(CH_3)$-$C(O)$-O-CH_2-CF_2-CFH-CF_3 (> 10.000), CH_2=$C(CH_3)$-$C(O)$-O-CH_2-CF_2-CF_2H (> 10.000), CF_3CF_2-CF_2-$CH(CF_3)_2$ (<250),



$C(CF_3)_2$ (< 100), $C_8F_{17}OSO_2F$ (< 50 g/m^3).

Our results prove that it is possible to predict the order of LC_{50} values with surprising accuracy and little experimental effort.