

Calculation Of Drug Lipophilicity The Hydrophobic Fragmental Constant Approach

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Due to the importance of lipophilicity, different ways to assess the value experimentally and to calculate $\log P$ have been developed: the shake flask method, chromatography, 55 or pH titration 56 are routinely used to obtain experimental

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CONCEPT OF CLEARANCE

Calculation Of Drug Lipophilicity The

$$LiPE = pIC_{50} + \log P$$

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In addition to the ALOGPS 2.1 logP and logW it also displays values calculated with Pharma Algorithms LogP, LogS and pKa, Actelion LogP & LogS (many thanks to Dr Thomas Sander), Molinspiration logP, KOWWIN logP, ALOGP (Viswanadhan et al, 1989), MLOGP (Moriguchi et al, 1992) implemented in

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