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Formulation; 2.2.2 Model Equations; 2.2.3 Model Parameterization; 2.2.4 Model Calculations; 2.3 Experimental Methods Demonstrated for Groups of Chemicals; 2.4 PBPK Models for Halogenated Alkanes; 2.4.1 Anesthetic Gases
2.4.2 Chlorofluorocarbons (CFCs), Refrigerants, and Halons2.4.3 Halogenated Alkanes; 2.5 Summary; Notation; References; CHAPTER 3 HALOGENATED ALKENES; 3.1 Introduction; 3.2 The Chloroethylenes: Background; 3.3 Review of PBPK Models; 3.3.1 Vinyl Chloride (VC); 3.3.2 Vinyl Fluoride (VF); 3.3.3 cis-1,2-Dichloroethylene (cDCE) and trans-1,2-Dichloroethylene (tDCE); 3.3.4 Vinylidene Chloride (VDC); 3.3.5 Trichloroethylene (TCE); 3.3.6 Tetrachloroethylene (PERC); 3.3.7 Allyl Chloride (AC); 3.3.8 b-Chloroprene (CD); 3.3.9 Hexachlorobutadiene, HCB; 3.4 Summary; Notation; References CHAPTER 4 ALKENE AND AROMATIC COMPOUNDS4.1 Introduction; 4.2 PK and Pharmacodynamic Properties Important in PBPK Model Development for Aromatic and Alkene Compounds; 4.2.1 Metabolism and Mode of Action; 4.2.2 Model Structures; 4.2.3 PK Differences; 4.2.4 Extrahepatic Metabolism and Transport of Metabolites; 4.2.5 GSH Conjugation; 4.2.6 Endogenous Production; 4.2.7 Reactivity with DNA and Protein; 4.2.8 Inhibition of Second Oxidative Steps; 4.2.9 Variability and PK Differences; 4.2.10 Subcompartments in PBPK Models; 4.2.11 "Privileged Access" of Epoxide Hydratase to Epoxide Substrates
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5.3 Creating the Air-Phase Compartments

Sommario/riassunto

A definitive, single source of information on PBPK modelingPhysiologically-based pharmacokinetic (PBPK) modeling is becoming increasingly important in human health risk assessments and in supporting pharmacodynamic modeling for toxic responses. Organized by classes of compounds and modeling purposes so users can quickly access information, this is the first comprehensive reference of its kind.This book presents an overview of the underlying principles of PBPK model development. Then it provides a compendium of PBPK modeling information, including historical development, specific modeli