```
parameterize_SteadyState <- function(chem.CAS=NULL,chem.name=NULL,species="Human")
{
  if (is.null(chem.CAS) & is.null(chem.name))
  {
    stop("Must specifiy compound name or CAS.\n")
  } else if ((!is.null(chem.CAS) & !any(chem.invivo.PK.data$CAS==chem.CAS)) & (!is.null(chem.name) &
!any(chem.invivo.PK.data$Compound==chem.name)))
  {
    stop("Compound not found.\n")
  }

  if (!is.null(chem.CAS))
  {
    this.chem.data <- subset(chem.invivo.PK.data,CAS==chem.CAS)
    chem.name <- this.chem.data[1,"Compound"]
  } else {
    this.chem.data <- subset(chem.invivo.PK.data,Compound==chem.name)
    chem.CAS <- this.chem.data[1,"CAS"]
  }

  if (!(species %in% colnames(PK.physiology.data)))
  {
    if (toupper(species) %in% toupper(colnames(PK.physiology.data)))
    {
      PK.phys.species <-
colnames(PK.physiology.data)[toupper(colnames(PK.physiology.data))==toupper(species)]
      warning(paste(species,"coerced to",PK.phys.species,"for physiological data."))
    } else stop(paste("Physiological PK data for",species,"not found."))
  } else PK.phys.species <- species
  this.phys.data <- PK.physiology.data[,PK.phys.species]
  names(this.phys.data) <- PK.physiology.data[,1]
  #mL/min:
  QGFRc <- this.phys.data["GFR"]
  BW <- this.phys.data["Average BW"]

  if (!(paste(species,"Vol (L/kg)") %in% colnames(tissue.data)))
  {
    if (toupper(paste(species,"Vol (L/kg)")) %in% toupper(colnames(tissue.data)))
    {
      tissue.vols <- tissue.data[,toupper(colnames(tissue.data))==toupper(paste(species,"Vol (L/kg)"))]
      tissue.flows <- tissue.data[,toupper(colnames(tissue.data))==toupper(paste(species,"Flow
(mL/min/kg)"))]
      warning(paste(species,"coerced to",toupper(species),"for physiological data."))
    } else stop(paste("Tissue data for",species,"not found."))
  } else {
    tissue.vols <- tissue.data[,paste(species,"Vol (L/kg)")]
    tissue.flows <- tissue.data[,paste(species,"Flow (mL/min/kg)")]
  }
  names(tissue.vols) <- tissue.data[,1]
  names(tissue.flows) <- tissue.data[,1]
  #mL/min:
  Qhc <- tissue.flows["Liver"]
  liver.volume.per.kgBW <- tissue.vols["Liver"]

  #Want the units of uL/min/10^6 hepatocytes
  CLint <- get_invitroPK_param("Clint",species,chem.CAS=chem.CAS)
```

```
  fub <- get_invitroPK_param("Fub",species,chem.CAS=chem.CAS)
  if (fub == 0)
  {
    fub <- 0.005
    warning("Fraction unbound = 0, changed to 0.005.")
  }

  Params <- list()
  Params[["CLint"]] <- CLint # uL/min/10^6
  Params[["fub"]] <- fub # unitless fraction
  Params[["Qhc"]] <- Qhc/1000*60     #        L/h/kgBW
  Params[["QGFRc"]] <- QGFRc/1000*60 #        L/h/kgBW
  Params[["BW"]] <- BW # kg
  Params[["MW"]] <- get_physchem_param("MW",chem.CAS=chem.CAS) # molecular weight g/mol
  Params[["million.cells.per.gliver"]] <- 110 # 10^6 cells/g-liver
  Params[["liver.volume.per.kgBW"]] <- liver.volume.per.kgBW # L/kg BW
  Params[["tissue.density"]] <- 1.05 # g/mL
 # Params[["CLmetabolism"]] <- calc_Hepatic_Clearance(Params)
  return(Params)
}
```