Descriptions taken from EPA's 'httk' R package documentation

Variable Name	Description	Units
Compound	Name of chemical compound	
CAS	Chemical Abstracts Service Registry Number	
CAS.Checksum	Is CAS valid?	
DTXSID	DSSTox Structure ID	
Formula	The proportions of atoms within the chemical compound	
All.Compound.Names	All names of chemical as they occur in the data	
logHenry	The log10 Henry's law constant	log10(atmosphers*m^3/mole)
logHenry.Reference	Reference for logHenry	
logMA	The log10 phospholipid water partition coefficient (PC) or "Membrane affinity"	log10 unitless ratio
logMA.Reference	Reference for logMA	
logP	The log10 octanol:water PC	log10 unitless ratio
logP.Reference	Reference for logP	
logPwa	The log10 water:air PC	log10 unitless ratio
logPwa.Reference	Reference for logPwa	
logWSol	The log10 water solubility	log10 (mole/L)
logWSol.Reference	Reference for logWSol	
MP	The chemical compound melting point	Degrees celcius
MP.Reference	Reference for MP	
MW	The chemical compound molecular weight	g/mol
MW.Reference	Reference for MW	
pKa_Accept	The hydrogen acceptor equilibria concentrations; basic association constant	Logarithm
pKa_Accept.Reference	Reference for pKa_Accept	
pKa_Donor	The hydrogen donor equilibria concentrations; acid disassociation constant	Logarithm
pKa_Donor.Reference	Reference for pKa_Donor	
All.Species	All species for which data were available	
Dog.Foral	Dog in vivo measured fractional systemic bioavailabiliy of an oral dose, modeled as the product of Fabs*Fgut*Fhep	unitless fraction
Dog.Foral.Reference	Reference for Dog.Foral	
DTXSID.Reference	Reference for DTXSID	
Formula.Reference	Reference for Formula	
Human.Caco2.Pab	Human Caco-2 Apical-to-Basal Membrane Permeability	10^-6 cm/s
Human.Caco2.Pab.Reference	Reference for Human.Caco2.Pab value	
Human.Clint	Human (Primary hepatocyte suspension) intrinsic hepatic clearance. Entries with comma separated values are Bayesian estimates of the Clint distribution - displayed as the median, 95th credible interval (that is quantile 2.5 and 97.5, respectively), and p-value.	uL/min/10^6 (hepatocytes)
Human.Clint.pValue	Human probability that there is no clearance observed. Values close to 1 indicate clearance is not statistically significant.	None
Human.Clint.pValue.Reference	Reference for Human.Clint.pValue value	
Human.Clint.Reference	Reference for Human.Clint value	
Human.Fabs	Human in vivo measured fraction of an oral dose of chemical absorbed from the gut lumen into the gut	Unitless fraction
Human.Fabs.Reference	Reference for Human.Fabs value	
Human.Fgut	Human In vivo measured fraction of an oral dose of chemical that passes gut metabolism and clearance	Unitless fraction
Human.Fgut.Reference	Reference for Human.Fgut value	
Human.Fhep	Human first pass hepatic metabolism	Unitless fraction
Human.Fhep.Reference	Reference for Human.Fhep value	
Human.Foral	Human in vivo measured fractional systemic bioavailabiliy of an oral dose, modeled as the product of Fabs*Fgut*Fhep	Unitless fraction
Human.Foral.Reference	Reference for Human.Foral value	
Human.Funbound.plasma	Chemical fraction unbound in presence of plasma proteins (fup). Entries with comma separated values are Bayesian estimates of the fup distribution - displayed as the median and 95th credible interval (that is quantile 2.5 and 97.5, respectively).	Unitless fraction
Human.Funbound.plasma.Reference	Reference for Human.Funbound.plasma value	
Human.Rblood2plasma	Human chemical concentration blood to plasma ratio	Unitless ratio
Human.Rblood2plasma.Reference	Reference for Human.Rblood2plasma value	
Monkey.Foral	Monkey in vivo measured fractional systemic bioavailabiliy of an oral dose, modeled as the product of Fabs*Fgut*Fhep	Unitless fraction
Monkey.Foral.Reference	Reference for Monkey.Foral value	
Mouse.Foral	Mouse in vivo measured fractional systemic bioavailabiliy of an oral dose, modeled as the product of Fabs*Fgut*Fhep	Unitless fraction
Mouse.Foral.Reference	Reference for Mouse.Foral value	
Mouse.Funbound.plasma	Mouse chemical fraction unbound in presence of plasma proteins (fup). Entries with comma separated values are Bayesian estimates of the fup distribution - displayed as the median and 95th credible interval (that is quantile 2.5 and 97.5, respectively).	Unitless fraction
Mouse.Funbound.plasma.Reference	Reference for Mouse.Funbound.plasma value	
Rabbit.Funbound.plasma	Rabbit chemical fraction unbound in presence of plasma proteins (fup). Entries with comma separated values are Bayesian estimates of the fup distribution - displayed as the median and 95th credible interval (that is quantile 2.5 and 97.5, respectively).	Unitless fraction
Rabbit.Funbound.plasma.Reference	Reference for Rabbit.Funbound.plasma value	
Rat.Clint	Rat (Primary hepatocyte suspension) intrinsic hepatic clearance. Entries with comma separated values are Bayesian estimates of the Clint distribution - displayed as the median, 95th credible interval (that is quantile 2.5 and 97.5, respectively), and p-value.	uL/min/10^6 (hepatocytes)
Rat.Clint.pValue	Rat probability that there is no clearance observed. Values close to 1 indicate clearance is not statistically significant.	None
Rat.Clint.pValue.Reference	Reference for Rat.Clint.pValue value	
Rat.Clint.Reference	Reference for Rat.Clint value	
Rat.Foral	Rat in vivo measured fractional systemic bioavailabiliy of an oral dose, modeled as the product of Fabs*Fgut*Fhep	Unitless fraction
Rat.Foral.Reference	Reference for Rat.Foral value	
Rat.Funbound.plasma	Rat chemical fraction unbound in presence of plasma proteins (fup). Entries with comma separated values are Bayesian estimates of the fup distribution - displayed as the median and 95th credible interval (that is quantile 2.5 and 97.5, respectively).	Unitless fraction
Rat.Funbound.plasma.Reference	Reference for Rat.Funbound.plasma value	
Rat.Rblood2plasma	Rat chemical concentration blood to plasma ratio	Unitless ratio
Rat.Rblood2plasma.Reference	Reference for Rat.Rblood2plasma value	
SMILES.desalt.Reference		
Chemical.Class	All classes to which the chemical has been assigned	