| **USER INTERFACE** | **INTERNAL** | **TECH DOC** | **DESCRIPTION** | **UNITS** |
| --- | --- | --- | --- | --- |
|  | **ChemicalRecord** | **Chemical Underlying Data** | **For each chemical simulated, the following Parameters are required** |  |
| Chemical | ChemName | N / A | Chemical's Name. Used for Reference only. | N / A |
| CAS Registry No. | CASRegNo | N / A | CAS Registry Number. Used for Reference only. | N / A |
| Molecular Weight | MolWt | MolWt | Molecular weight of pollutant | g/mol |
| Dissociation Constant | pka | pKa | Acid dissociation constant | negative log |
| Henry's Law Constant | Henry | Henry | Henry's law constant | atm m3 mol-1 |
| Octanol-water partition coefficient | LogKow | LogKow | Log octanol-water partition coefficient | unitless |
| KPSED | KPSed | KPSed | Detritus-water partition coefficient | L/kg OC |
| KOMRefrDOM | KOMRefrDOM | KOMRefrDOM | Reftractory DOM to Water Partition Coefficient | L/kg OM |
| Uptake Rate (K1) Detritus | K1Detritus | K1Detr | Uptake rate constant for organic matter, default of 1.39 | L/kg dry day |
| Activation Energy for Temperature | En | En | Arrhenius activation energy | cal/mol |
| Rate of Anaerobic Microbial Degradation | KMDegrAnaerobic | KAnaerobic | Decomposition rate at 0 g/m3 oxygen | 1/d |
| Max. Rate of Aerobic Microbial Degradation | KMDegrdn | KMDegrdn | Maximum (microbial) degradation rate | 1/d |
| Uncatalyzed hydrolysis constant | KUnCat | KUncat | The measured first-order reaction rate at ph 7 | 1/d |
| Acid catalyzed hydrolysis constant | KAcid | KAcid | Pseudo-first-order acid-catalyzed rate constant for a given ph | L/mol ∙ d |
| Base catalyzed hydrolysis constant | KBase | KBase | Pseudo-first-order rate constant for a given ph | L/mol ∙ d |
| Photolysis Rate | PhotolysisRate | KPhot | Direct photolysis first-order rate constant | 1/d |
| Weibull Shape Parameter | Weibull\_Shape | Shape (Internal Model) | Parameter expressing variability in toxic response; default is 0.33 | unitless |
| Chemical is a Base | ChemIsBase | Compound is a base | True if the compound is a base | True/False |
| This Chemical is a PFA | IsPFA | Compound is a PFA | True if the compound is a perfluorinated surfactant | True/False |
| Type of PFA | PFAType | carboxylate / sulfonate | Sulfonate group and carboxylate group | carboxylate / sulfonate |
| Kom for Sediments (PFA) | PFASedKom | Kom for Sediments | Organic matter partition coefficient for the PFA | L/kg |
| Use BCF to Estimate Uptake | BCFUptake |  |  |  |