What is new in ECOSAR 2.0?

The ECOSAR user interface was updated using Java coding and JChemPaint for chemical structure viewing, drawing, and importing. In addition, several chemical classes were updated since the last version of ECOSAR was released (ECOSAR V1.11). The chemical classes in ECOSAR V2.0 with updated QSARs based on new data or revised definition sheets are listed below:

ECOSAR V2.0 Updates

Class Name	ECOSAR V2.0 Updated QSARs	Update details
Acrylates	X	
Aldehydes (mono)	X	
Amides	X	
Anilines (hindered)	X	
Anilines (unhindered)	X	
Benzotriazoles	X	
Benzyl Halides	X	
Benzyl Nitriles	X	
Carbamate Esters	X	
Carbonyl Ureas	X	
Esters	X	
Esters, Dithiophosphate	X	
Esters, Monothiophosphate	X	
Esters, Phosphates-Inert Substitutions	X	New class: sub-classification of Esters, Phosphates class
Esters, Phosphates-Withdrawing Substitutions	X	New class: sub-classification of Esters, Phosphates class
Esters, Phosphinates	X	
Haloalcohols	Deleted	-Measured data from this class will be moved to the Neutral Organics class in the next version update
Halo Ketones	X	
Hydrazines	X	
Imides	X	
Ketone Alcohols	X	
Methacrylates	X	

Nitro Alcohols	X	
Oxetanes	X	
Peroxides		Definition sheet updated
Peroxy Acids	X	Definition sheet updated
Peroxy Esters		Definition sheet updated
Polyaliphatic Nitriles	X	
Pyrroles/Diazoles	X	New class: combined Imidazoles & Pyrazoles-Pyrroles classes
Pyridine-α-acid	X	
Substituted Ureas	X	
Thiophenes	X	
Thiotetrazoles	X	
Thioureas	X	
Triazines, Aromatic	X	
Triazoles (non-fused)	X	
Vinyl/Allyl /Propargyl Alcohols Unhindered	X	New class: combined Unhindered Vinyl/Allyl Alcohols & Propargyl Alcohols
Vinyl/Allyl/ Propargyl Alcohols Hindered	X	New class: combined Hindered Vinyl/Allyl Alcohols & Propargyl Alcohols
Vinyl/allyl/Propargyl Aldehydes Hindered	X	New class: previously Vinyl/Allyl Aldehydes (split into hindered and unhindered)
Vinyl/allyl/Propargyl Aldehydes Unhindered	X	New class: previously Vinyl/Allyl Aldehydes (split into hindered and unhindered)
Vinyl/Allyl/Propargyl Esters	X	New class: previously Vinyl/Allyl Esters
Vinyl/Allyl/Propargyl Ethers	X	New class: combined Vinyl/Allyl Ethers & Propargyl Ethers
Vinyl/Allyl/Propargyl Halides	X	New class: combined Vinyl/Allyl Halides & Propargyl Halides
Vinyl/allyl/Propargyl Ketones	X	New class: previously Vinyl/Allyl Ketones
Vinyl/Allyl/ Propargyl Aromatic Amines	X	New class: previously Vinyl/Allyl Pyrazoles-Pyrroles
Vinyl/Allyl/ Propargyl Nitriles	X	New class: previously Vinyl/Allyl Nitriles
Vinyl/Allyl/Propargyl Sulfones	X	New class: previously Vinyl/Allyl Sulfones
Special Classes		
Surfactants, nonionic	X	
Polymers, nonionic	X	
Polymers, anionic	X	
Polymers, cationic	X	
Polymers, amphoteric	X	