Semi-explicit

Triple bonds are treated as CH and C “olefin” cases

The phenyl group is used to derive an “aromatic” offset for CH and C olefin values, such that, with the “six-membered ring” added, equivalent volumes for benzene is calculated

Halogen doubles and triples for delta-p do not include vicinal substitution patterns

For bromine and iodine single substitutions, cycloaliphatic values are treated as aliphatic

For ethers, ketones, aldehydes, esters, acids, and nitriles – “aromatic” refers to any one vicinal carbon, as does “cycloaliphatic” (by default this includes ‘in-ring’ cases too)

‘gem’ and ‘vicinal’ diols are coded as separate corrections applied to the alcohol group

The “>NH2 amine” group is interpreted as referring to secondary amines (tertiary amines assumed to contribute zero)

The “>NH amide” group (the only amide group) is interpreted as referring to any H-containing amide

Phosphorous-containing groups not implemented

“>C=” includes allenes (no separate group)

‘?’ entries on the table default to “alkane”, or, “cycloalkane”, or to scaled value of the next lowest homolog if no alkane value is provided (e.g. values for I3 are 1.5 \* the reported value for I2

Implicit

Anhydride groups are treated as 1.5 ester groups

Composite group examples: urea ?, urethane ?

Additional validations:

Gem-diol

Fixes:

-PO4

-Formaldehyde

-ketone group names with zero for O