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

The “=PO2 ester” group is interpreted to exclude PO4 structures

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

‘?’ entries on the table default to “alkane”, 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) – applies to halogens only

Implicit

Anhydride groups are treated as 1.5 ester groups

Composite group examples: urea ?, urethane ?

Additional validations:

Gem-diol