

## Calculation of biodiesel physicochemical properties from the composition of the fatty acids methylesters

The physicochemical properties of the mixtures of fatty acids methylesters were calculated using predictive equations (above) and database values of individual pure fatty acids methylesters (below).  $c_i$  is the relative composition in mass, the subscript ( $i$ ) indicating each individual methylester.

### Mixtures of fatty acid methylesters

Property	Equation	References
Density at 15°C, g/L	$\rho_{mix} = \sum_i (c_i \cdot \rho_i)$	41,45
Kinematic Viscosity at 40°C, mm <sup>2</sup> /s	$\nu_{mix} = \sum_i (c_i \cdot \nu_i)$	41,46
Saponification Number	$SN_{mix} = \sum_i (c_i \cdot 560) / MW_i$	41
Iodine Number	$IV_{mix} = \sum_i (c_i \cdot D_i \cdot 254) / MW_i$	41
Cetane Number	$CN_{mix} = 1.068 \cdot \sum_i (c_i \cdot CN_i) - 6.747$	41,47
Higher Heating Value, MJ/Kg	$HHV_{mix} = 49.43 - (0.041 \cdot SN_{mix} + 0.015 \cdot IV_{mix})$	48
Flash Point, °C	$FP_{mix} = (HHV_{mix} - 32.12) / 0.021 - 273.15$	48

### Individual fatty acid methylesters

Property		C16	C16:1	C18	C18:1	C18:2	C18:3	References
Double bonds	$D_i$	0	1	0	1	2	3	
Molecular weight, g/mol	$\rho_i$	270.5	268.4	298.5	296.5	294.5	292.5	
Cetane Number	$CN_i$	74.3	51.0	75.6	56.5	38.2	22.7	47
Density at 15°C, g/L	$\rho_i$	864.2	882.4	867.6	877.5	893.2	901.8	45
Kinematic viscosity at 40°C, mm <sup>2</sup> /s	$\nu_i$	4.4	3.7	5.9	4.5	3.7	3.1	46