Substance: Dimethyl terephthalate

HTSUS item number of substance: 2917.37.00.00
CAS number of substance: 120-61-6
Schedule B number of substance: 2917.37.0000

Predominant method of production: Dimethyl terephthalate is produced by the esterification of terephthalic acid with methanol. Terephthalic acid is made from p-xylene (an isomer of xylene) and oxygen. Methanol is made from syngas. Hydrogen for the syngas is made from methane via the steam methane reforming process.

The chemical equation for the production of dimethyl terephthalate is:
$C_8H_6O_4$ (terephthalic acid) + 2 CH_3OH (methanol) → $C_{10}H_{10}O_4$ (dimethyl terephthalate) + 2 H_2O (water)

Derived taxable chemicals:

Terephthalic acid is made from p-xylene and oxygen:
C_8H_{10} (xylene) + 3 O_2 → $C_8H_6O_4$ (terephthalic acid) + 2 H_2O

Methanol is made from syngas:
2 [CO + 2H_2 → CH_3OH (methanol)]

Hydrogen is made from steam-methane reforming:
CH_4 (methane) + 2 H_2O → 4 H_2 (hydrogen) + CO_2

Xylene and methane are taxable chemicals. Therefore, the derived stoichiometric material consumption equation is:
[C_8H_{10} (xylene) + 3 O_2 - 2 H_2O] + [2 CO +(CH_4 (methane) + 2 H_2O - CO_2)] → $C_{10}H_{10}O_4$ (dimethyl terephthalate) + 2 H_2O

Simplifying to the stoichiometric material consumption equation:
C_8H_{10} (xylene) + CH_4 (methane) + 3 O_2 + 2 CO → $C_{10}H_{10}O_4$ (dimethyl terephthalate) + 2 H_2O + CO_2

Stoichiometric material consumption equation for dimethyl terephthalate:

C_8H_{10} (xylene) + CH_4 (methane) + 3 O_2 + 2 CO → $C_{10}H_{10}O_4$ (dimethyl terephthalate)+ 2 H_2O + CO_2

Stoichiometric material consumption equation used to determine the weight (in grams) of materials used to produce dimethyl terephthalate:						
C_8H_{10} (xylene) + CH_4 (methane)	+	3 O_2 + 2 CO	→	$C_{10}H_{10}O_4$	+	2 H_2O + CO_2
106.16 g + 16.06 g = 122.22 g		96.00 g + 56.02 g = 152.02 g		194.19 g		

Total Weight = 122.22 g + 152.02 g = 274.24 g

Percent of dimethyl terephthalate produced with taxable chemicals:
(122.22 g Tax Weight) / (274.24 g Total Weight) x 100% = 44.57%

Conversion factors of taxable chemicals: The weight of an individual taxable chemical used in the stoichiometric material consumption equation is divided by the weight of the substance. This ratio is a multiplier, i.e. a *conversion factor*, that is used for each taxable chemical used in the predominant method of production of the substance to determine an overall tax rate for the substance.

For example:
If: Taxable chemical A + Taxable chemical B → Substance X

Then: A conversion factor = (Chemical Weight A) / (Chemical Weight X)

B conversion factor = (Chemical Weight B) / (Chemical Weight X)

C_8H_{10} (p-xylene) + CH_4 (methane) + 3 O_2 + 2 CO → $C_{10}H_{10}O_4$ (dimethyl terephthalate) + 2 H_2O + CO_2

Both p-xylene and methane are taxable chemicals.

Conversion factor p-xylene: (106.16 g p-xylene) / (194.19 g dimethyl terephthalate) = 0.55

Conversion factor methane: (16.06 g methane) / (194.19 g dimethyl terephthalate) = 0.08

In summary, dimethyl terephthalate should be added to the list of taxable substances and p-xylene and methane are the taxable chemicals used to produce dimethyl terephthalate.

Percent Composition Taxable	44.57 %
Conversion factor for p-xylene	0.55
Conversion factor for methane	0.08

The tax rate for dimethyl terephthalate is calculated as follows: [($9.74 rate of tax for p-xylene) x 0.55] + [($6.88 rate of tax for methane) x 0.08]

Total tax rate for dimethyl terephthalate = $5.91 per ton