

Some of the partial speciation profiles that come with version 4.09D do not work. When the program was updated, two of the chemical names were changed. The names were not changed in the profiles. To use the profiles correctly you can 'add' the two chemicals to the chemical database.

Open the TANKS program. Close the TANK Record window.

To update the chemical data, open the DATA menu and select CHEMICAL/EDIT DATABASE.

This opens the chemical data window. Click on ADD NEW at the lower left of the window.

Add isooctane CAS 00540-84-1
Density - 5.76
Weight - 114.23
Vapor pressure at 60F is 0.596115
Antoine's coefficients:
A: 6.8118
B: 1257.84
C: 220.74

SAVE the chemical

Add ethanol CAS 00064-17-5
Density - 6.61
Weight - 46.07
Vapor Pressure

Degrees F	VP
40	0.193
50	0.406
60	0.619
70	0.87
80	1.218
90	1.682
100	2.32

SAVE the chemical, answer NO to Add New and close the chemical data window. The partial speciation profiles will now appear correctly.

Chemical

Chemical Name:

Ethanol

CAS Number:

00064-17-5

Category:

Organic Liquids

Liq. Mol. Weight:

46.07

Liquid Density (lb/gal @ 60F):

6.61

Vapor Molecular Weight:

46.07

Vapor Pressure Information (fill in one or more options completely)

Option 1: Enter Vapor Pressure (psia) for each temperature:

40F: 0.193

80F: 1.218

50F: 0.406

90F: 1.682

60F: 0.619

100F: 2.32

70F: 0.87

Option 2: Constants for Antoine's Equation (using C)

A: 8.321

B: 1718.21

C: 237.52

Option 3: Constants for Antoine's Equation (using K)

A: 0

B: 0

Option 4: Reid Vapor Pressure (psia): (Distillates, Crude Oil)

0

ASTM Slope: (Distillates Only)

0

Add New

Delete

Save

Close

Help

Chemical Name:

Isooctane

CAS Number:

00540-84-1

Category:

Organic Liquids

Liq. Mol. Weight:

114.23

Liquid Density (lb/gal @ 60F):

5.76

Vapor Molecular Weight:

114.23

Vapor Pressure Information (fill in one or more options completely)

Option 1: Enter Vapor Pressure (psia) for each temperature:

40F:

0

80F:

0

50F:

0

90F:

0

60F:

0.596115

100F:

0

70F:

0

Option 2: Constants for Antoine's Equation (using C)

A:

6.8118

B:

1257.84

C:

220.74

Option 3: Constants for Antoine's Equation (using K)

A:

0

B:

0

Option 4: Reid Vapor Pressure (psia): (Distillates, Crude Oil)

0

ASTM Slope: (Distillates Only)

0

Add New

Delete

Save

Close

Help