根据CAS号, 从数据库中找到对应物质的物性数据以苯为例子, CAS = 71-43-2

• Pc, 临界压力, Pa

Pc = 4895000

• Tc, 临界温度, K

Tc = 562.0500

• Vc,临界体积, <u>m³</u> kmol

Vc = 0.2560

• Zc, 临界压缩因子, -

Zc = 0.2680

• Tb, 常压沸点温度, K

Tb = 353.2400

• Ttriple, 三相点温度, K

Ttriple = 278.6800

• Ptriple, 三相点压力, Pa

Ptriple = 4.7642e+03

• Mw,摩尔质量,kg kmol

Mw = 78.1140

ω,偏心因子,-

Omega = 0.2090

• H^{m}_{form} ,标准摩尔生成焓, $\frac{J}{kmol}$

Hfrom = 82880000

• G^{m}_{fron} , 标准摩尔生成自由能, $\frac{J}{kmol}$

Gform = 129600000

• LiquidDensity,液体的密度, $\frac{\text{kmol}}{m^3}$

$$\rho_L = \frac{A}{B^{\left(1 + \left(1 - \frac{T}{C}\right)^D\right)}}, \quad T \in [\mathsf{Tmin}, \mathsf{Tmax}]$$

