

# Memo

## User guide

Thermotools

Location:  
Trondheim  
NORWAY

<https://thermotools.github.io/thermopack/index.html>

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**AUTHOR**  
Vegard Gjeldvik Jervell, Morten Hammer

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## 1 Introduction

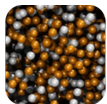
This document is intended for generic user documentation. Also see <https://github.com/SINTEF/thermopack/wiki>.

## 2 Phase keys

The phase keys are defined in `src/thermopack_constants.f90`, and are shown in Table 1.

Phase	Key	Description
Two-phase	0	Liquid-vapor two-phase mixture (Code: TWOPH)
Liquid	1	Single phase liquid (Code: LIQPH)
Vapor	2	Single phase vapor (Code: VAPPH)
Minimum Gibbs	3	Single phase root with the minimum Gibbs free energy (Code: MINGIBBSPH)
Single	4	Single phase not identified as liquid or vapor (Code: SINGLEPH)
Solid	5	Single phase solid (Code: SOLIDPH)
Fake	6	In rare cases no physical roots exist, and a fake liquid root is returned (Code: FAKEPH)

**Table 1:** Phase flags in thermopack.



### 3 Cubic Equations of State

Name	Key
Van der Waal	VdW
Soave Redlich Kwong	SRK
Peng Robinson	PR
Schmidt-Wensel	SW
Patel Teja	PT
Translated consistent PR	tcPR

**Table 2:** Cubic Equations of state implemented in ThermoPack and the corresponding keys used for initialization.

#### 3.1 Pure fluid $\alpha$

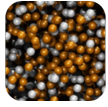
Model	Key
Model default*	Classic
Twu-Coon-Bluck-Cunningham	TWU
Mathias-Copeman	MC
Graboski and Daubert	GD
Redlich-Kwong	RK
Soave	Soave
Peng Robinson 76	PR
UMR $\alpha$ formulation	UMR
Peng Robinson 78	PR78
Van der Waal	VdW
Schmidt-Wensel	SW
Patel Teja	PT

\*Will use original  $\alpha$  for specified EOS.  
E.g. SRK will use Soave  $\alpha$ ,  
Peng-Robinson will use PR  $\alpha$  etc.

#### 3.2 $\alpha$ mixing Rules

Name	Key
Van der Waals	Classic or vdW
Wong Sandler	WS
Huron Vidal	HV or HV2
NRTL	NRTL
UNIFAC	UNIFAC

**Table 3:** Mixing rules and phases available in thermopack, with the corresponding keys used to identify them.



## 4 Adding new fluids

The fluid database consists of a set of `.json`-files in the `fluids` directory. These files are used to auto-generate the FORTRAN-files `compdatadb.f90` and `saftvmie_datadb.f90` by running the respective python scripts `compdata.py` and `saftvmie.py` found in the directory `addon/pyUtils/datadb/`. The files are generated in the current working directory and must be copied to the `src`-directory before recompiling ThermoPack to make the fluids available.

A `<fluid>.json` file must contain a minimal set of data to be valid. This includes the critical point, accentric factor, mole weight and ideal gas heat capacity.

### 4.1 Ideal gas heat capacity

Several different correlations for the heat capacity are available, selected by the "correlation"-key in the "ideal-heat-capacity-1" field of the fluid files. These are summarized in Table 4.

**Table 4:** Ideal gas heat capacity correlations, and the corresponding keys used in the fluid-database.

Key	Correlation	Equation	Unit
1	Sherwood, Reid & Prausnitz <sup>(a)</sup>	$A + BT + CT^2 + DT^3$	$\text{cal g}^{-1} \text{mol}^{-1} \text{K}^{-1}$
2	API-Project	44	-
3	Hypothetic components	-	-
4	Sherwood, Reid & Prausnitz <sup>(b)</sup>	$A + BT + CT^2 + DT^3$	$\text{J mol}^{-1} \text{K}^{-1}$
5	Ici (Krister Strøm)	$A + BT + CT^2 + DT^3 + ET^{-2}$	$\text{J g}^{-1} \text{K}^{-1}$
6	Chen, Bender (Petter Neksa)	$A + BT + CT^2 + DT^3 + ET^4$	$\text{J g}^{-1} \text{K}^{-1}$
7	Aiche, Daubert & Danner <sup>(c)</sup>	$A + B \left[ \frac{C}{T} \sinh \left( \frac{C}{T} \right) \right]^2 + D \left[ \frac{E}{T} \cosh \left( \frac{E}{T} \right) \right]^2$	$\text{J kmol}^{-1} \text{K}^{-1}$
8	Poling, Prausnitz & O'Connel <sup>(d)</sup>	$R (A + BT + CT^2 + DT^3 + ET^4)$	$\text{J mol}^{-1} \text{K}^{-1}$
9	Linear function and fraction	$A + BT + \frac{C}{T+D}$	$\text{J mol}^{-1} \text{K}^{-1}$
10	Leachman & Valenta for H <sub>2</sub>	-	-
11	Use TREND model	-	-
12	Shomate equation*	$A + BT_s + CT_s^2 + DT_s^3 + ET_s^{-2}$	$\text{J mol}^{-1} \text{K}^{-1}$

<sup>(a)</sup>3rd ed. <sup>(c)</sup>DIPPR-database

<sup>(b)</sup>4th ed. <sup>(d)</sup>5th ed.

\*Note:  $T_s = 10^{-3}T$