# Thermotools memo

**Thermotools**
Location:
Trondheim
NORWAY

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

## User guide

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## Contents



## 1 Introduction

This document is intended for generic user documentation. Also see https://github.com/thermotools/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-Cunninghan | 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 are used to auto-generate the FORTRAN-files compdatadb.f90 and saftvrmie_datadb.f90 by running the respective python scripts compdata.py and saftvrmie.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[(a)] | $A + BT + CT^2 + DT^3$ | $\mathrm{cal\,g^{-1}\,mol^{-1}\,K^{-1}}$ |
| 2 | API-Project | 44 | - |
| 3 | Hypothetic components | - | - |
| 4 | Sherwood, Reid & Prausniz[(b)] | $A + BT + CT^2 + DT^3$ | $\mathrm{J\,mol^{-1}\,K^{-1}}$ |
| 5 | Ici (Krister Strøm) | $A + BT + CT^2 + DT^3 + ET^{-2}$ | $\mathrm{J\,g^{-1}\,K^{-1}}$ |
| 6 | Chen, Bender (Petter Nekså) | $A + BT + CT^2 + DT^3 + ET^4$ | $\mathrm{J\,g^{-1}\,K^{-1}}$ |
| 7 | Aiche, Daubert & Danner[(c)] | $A + B\left[\frac{C}{T}\sinh\left(\frac{C}{T}\right)\right]^2 + D\left[\frac{E}{T}\cosh\left(\frac{E}{T}\right)\right]^2$ | $\mathrm{J\,kmol^{-1}\,K^{-1}}$ |
| 8 | Poling, Prausnitz & O'Connel[(d)] | $\mathrm{R}\left(A + BT + CT^2 + DT^3 + ET^4\right)$ | $\mathrm{J\,mol^{-1}\,K^{-1}}$ |
| 9 | Linear function and fraction | $A + BT + \frac{C}{T+D}$ | $\mathrm{J\,mol^{-1}\,K^{-1}}$ |
| 10 | Leachman & Valenta for $H_2$ | - | - |
| 11 | Use TREND model | - | - |
| 12 | Shomate equation* | $A + BT_s + CT_s^2 + DT_s^3 + ET_s^{-2}$ | $\mathrm{J\,mol^{-1}\,K^{-1}}$ |

[(a)]3rd ed. [(c)]DIPPR-database
[(b)]4th ed. [(d)]5th ed.
*Note: $T_s = 10^{-3}T$