

Memo

User guide

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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 α

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 α formulation	UMR
Peng Robinson 78	PR78
Van der Waal	VdW
Schmidt-Wensel	SW
Patel Teja	PT

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

3.2 α 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.