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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

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

3.1 Mixing Rules

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

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