

**substance: titanium oxide (TiO<sub>2</sub>)**

**property: thermodynamic parameters of phase transformation**

For general considerations on binary transition-metal compounds, on placement of d-bands and formal valence and on character of d-electrons, see , , . For a general characterization of titanium oxides, see document .

TiO<sub>2</sub> crystallizes in three polymorphic forms: anatase, brookite and rutile. Anatase and brookite transform to rutile if heated to 700°C and 900°C, respectively.

**thermodynamic parameters of phase transformation**

( $\Delta H_{tr}$ ,  $\Delta G_{tr}$  in kcal mol<sup>-1</sup>)

**anatase-rutile**

$\Delta H_{tr}^0$	+ 2.79	66V
	– 0.78(9)	79M
	– 1.57(19)	67N
	– 0.10(5)	61R
	+ 0.1	68R
$\Delta G_{tr}^0$	– 0.66	79M

**brookite-rutile**

$\Delta H_{tr}^0$	– 0.17(9)	79M
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Each phase consists of TiO<sub>6</sub> octahedra sharing four edges (anatase), three edges and a corner (brookite) or two edges and two corners (rutile)

**References:**

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