

zirconium

Other names:	zirconium element
Inchi:	InChI=1S/Zr
InchiKey:	QCWXUIWCKQGHC-UHFFFAOYSA-N
Formula:	Zr
SMILES:	[Zr]
Mol. weight [g/mol]:	91.22
CAS:	7440-67-7

Physical Properties

Property code	Value	Unit	Source
ea	0.43 ± 0.01	eV	NIST Webbook
ie	6.63 ± 0.00	eV	NIST Webbook
ie	6.63	eV	NIST Webbook
ie	6.63 ± 0.00	eV	NIST Webbook
ie	6.48 ± 0.07	eV	NIST Webbook
ie	5.80 ± 0.20	eV	NIST Webbook
ie	6.40 ± 0.10	eV	NIST Webbook
ie	6.84	eV	NIST Webbook
tt	1141.40	K	Thermophysical Properties of Solid Phase Zirconium at High Temperatures

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{\text{vap}}) = A + B/(T + C)$
Coeff. A	1.89892e+01
Coeff. B	-6.62535e+04
Coeff. C	-7.19000e+01
Temperature range (K), min.	2639.15
Temperature range (K), max.	4682.15

Sources

Thermodynamic properties of trizirconium tetraphosphate: Determination of the standard Gibbs free energies of formation of barium superionic solid electrolyte NPL Webbook:	https://www.doi.org/10.1016/j.jct.2004.11.002
The standard enthalpy of formation of superionic solid electrolyte	https://www.doi.org/10.1016/j.tca.2017.09.019
NPL Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7440677&Units=SI
The Yaws Handbook of Vapor Pressure: Thermophysical Properties of Solid Phase Zirconium at High Temperatures:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure-thermophysical-properties-of-solid-phase-zirconium-at-high-temperatures
	https://www.doi.org/10.1007/s10765-006-0080-z

Legend

ea:	Electron affinity
ie:	Ionization energy
p_{vap}:	Vapor pressure
tt:	Triple Point Temperature

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