

zirconium

Other names:	zirconium element
Inchi:	InChI=1S/Zr
InchiKey:	QCWXUUIWCKQGHC-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(Pvp) = 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

Determination of the standard Gibbs free energies of formation of barium zirconate and the temperature range of super ionic solid electrolyte NPL book:

<https://www.doi.org/10.1016/j.jct.2007.06.001>

<https://www.doi.org/10.1016/j.tca.2017.09.019>

<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
Thermodynamic properties of trizirconium tetraphosphate:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<https://www.doi.org/10.1007/s10765-006-0080-z>

<https://www.doi.org/10.1016/j.jct.2004.11.002>

Legend

ea: Electron affinity
ie: Ionization energy
pvap: Vapor pressure
tt: Triple Point Temperature

Latest version available from:

<https://www.chemeo.com/cid/48-844-2/zirconium.pdf>

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