

iron

Inchi:	InChI=1S/Fe
InchiKey:	XEEYBQQBJWHFJM-UHFFFAOYSA-N
Formula:	Fe
SMILES:	[Fe]
Mol. weight [g/mol]:	55.84
CAS:	7439-89-6

Physical Properties

Property code	Value	Unit	Source
affp	754.00	kJ/mol	NIST Webbook
basg	731.10	kJ/mol	NIST Webbook
ea	0.31 ± 0.20	eV	NIST Webbook
ea	0.15 ± 0.00	eV	NIST Webbook
ea	0.16 ± 0.04	eV	NIST Webbook
ea	0.14 ± 0.05	eV	NIST Webbook
ea	0.25 ± 0.20	eV	NIST Webbook
ie	7.92	eV	NIST Webbook
ie	7.90 ± 0.00	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
ie	7.87	eV	NIST Webbook
ie	7.90 ± 0.00	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
ie	7.70 ± 0.20	eV	NIST Webbook
ie	8.00 ± 0.50	eV	NIST Webbook
ie	7.87	eV	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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hvapt	408.60	kJ/mol	298.00	Thermodynamic activity measurements in nickel-base industrial alloys and steels by Knudsen cell Mass spectrometry
rhos	7849.00	kg/m3	293.00	Intercomparison of Thermophysical Property Measurements on Iron and Steels

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.72791e+01
Coeff. B	-3.73330e+04
Coeff. C	-1.84630e+02
Temperature range (K), min.	1708.15
Temperature range (K), max.	3133.35

Sources

Thermodynamic mixing effects of liquid ternary Au-Fe-Pd alloys by calorimetric method for determining the thermochemical energy storage capacities of redox metal oxides. *Chem. Eng. Sci.* 2012, 92, 1027-1035.

Heat capacity and thermodynamics of a synthetic two-line ferrihydrite, FeOOH. *Am. Mineral.* 2012, 97, 1027-1035.

Intercomparison of Thermophysical Property Measurements on Iron and Steels. *Thermophys. Prop.* 2010, 18, 1-10.

Correlation between excess volume and thermodynamic functions of liquid Pb-Fe, Cu-Fe, and Ni-Fe. *J. Chem. Eng. Data* 2018, 59, 1027-1035.

Determination of the standard molar enthalpies of formation and heat capacities of Dy + Fe binary system by double Knudsen cell mass spectrometry.

Thermodynamic activity measurements in nickel-base industrial alloys and steels by Knudsen cell mass spectrometry.

Thermodynamic measurement of Nd-Fe system by double Knudsen Cell Mass Spectrometry.

<https://www.doi.org/10.1016/j.tca.2012.02.012>

<https://www.doi.org/10.1016/j.tca.2019.01.008>

<https://www.doi.org/10.1016/j.tca.2006.02.029>

<https://www.thermochim.org/research/kdb/hcprop/showprop.php?cmpid=1952>

<https://www.doi.org/10.1016/j.jct.2012.11.012>

<https://www.doi.org/10.1007/s10765-019-2568-3>

<https://www.doi.org/10.1016/j.jct.2018.09.037>

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

<https://www.doi.org/10.1016/j.jct.2017.11.015>

<https://www.doi.org/10.1016/j.jct.2013.05.034>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C7439896&Units=SI>

<https://www.doi.org/10.1016/j.jct.2017.01.015>

<https://www.doi.org/10.1016/j.tca.2010.12.023>

Legend

affp:	Proton affinity
basg:	Gas basicity
ea:	Electron affinity
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
pvap:	Vapor pressure
rhos:	Solid Density

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