

Iron pentacarbonyl

Other names:	Fe(CO) ₅ Iron carbonyl Iron carbonyl (Fe(CO) ₅) Iron carbonyl (Fe(CO) ₅), (TB-5-11)- Pentacarbonyl iron
Inchi:	InChI=1S/5CO.Fe/c5*1-2;
InchiKey:	FYOFOKCECDGJBF-UHFFFAOYSA-N
Formula:	C ₅ FeO ₅
SMILES:	[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[Fe]
Mol. weight [g/mol]:	195.90
CAS:	13463-40-6

Physical Properties

Property code	Value	Unit	Source
affp	833.00	kJ/mol	NIST Webbook
basg	798.50	kJ/mol	NIST Webbook
chl	-1614.60 ± 6.30	kJ/mol	NIST Webbook
hf	-723.90 ± 6.70	kJ/mol	NIST Webbook
hfl	-764.10 ± 6.70	kJ/mol	NIST Webbook
hvap	38.10 ± 0.40	kJ/mol	NIST Webbook
hvap	40.20 ± 0.80	kJ/mol	NIST Webbook
ie	7.96 ± 0.02	eV	NIST Webbook
ie	8.00 ± 0.08	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	7.98 ± 0.01	eV	NIST Webbook
ie	8.40 ± 0.20	eV	NIST Webbook
ie	7.90 ± 0.03	eV	NIST Webbook
ie	7.95 ± 0.03	eV	NIST Webbook
tb	376.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	40.10 ± 0.50	kJ/mol	279.00	NIST Webbook
hvapt	39.00	kJ/mol	309.50	NIST Webbook
hvapt	37.60	kJ/mol	322.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.84775e+01
Coeff. B	-5.71116e+03
Coeff. C	3.59370e+01
Temperature range (K), min.	278.04
Temperature range (K), max.	397.85

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C13463406&Units=SI>

The Yaws Handbook of Vapor Pressure:

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

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature

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