

Nickelocene

Other names:	Bis(cyclopentadienyl)nickel (II) Bis(«eta»5-2,4-cyclopentadien-1-yl)nickel Di-«pi»-cyclopentadienylnickel Nickel, bis(«eta»5-2,4-cyclopentadien-1-yl)- Nickel, bis(«eta»5-cyclopentadienyl)- Nickel, compd with «pi»-cyclopentadienyl (1:2) Nickel, di-«pi»-cyclopentadienyl- Nickel, dicyclopentadienyl- Nikelocen bis(.eta.5-2,4-cyclopentadien-1-yl)nickel bis(cyclopentadienyl)nickel(II) bis(«eta»5-Cyclopentadienyl) nickel dicyclopentadienylnickel «pi»-Cyclopentadienyl compd. with nickel
Inchi:	InChI=1S/2C5H5.Ni/c2*1-2-4-5-3-1;/h2*1-5H;
InchiKey:	FOOKRXHSBKEWSE-UHFFFAOYSA-N
Formula:	C10H10Ni
SMILES:	C12C3C4C5C1[Ni]23451678C2C1C6C7C28
Mol. weight [g/mol]:	188.88
CAS:	1271-28-9

Physical Properties

Property code	Value	Unit	Source
affp	935.70	kJ/mol	NIST Webbook
basg	907.30	kJ/mol	NIST Webbook
chs	-5878.50 ± 4.20	kJ/mol	NIST Webbook
chs	-5889.40 ± 1.70	kJ/mol	NIST Webbook
chs	-5627.90 ± 2.50	kJ/mol	NIST Webbook
hf	346.10 ± 4.50	kJ/mol	NIST Webbook
hf	333.50 ± 3.10	kJ/mol	NIST Webbook
hf	357.00 ± 2.30	kJ/mol	NIST Webbook
hf	335.20 ± 2.90	kJ/mol	NIST Webbook
hfs	274.60 ± 4.40	kJ/mol	NIST Webbook
hfs	262.00 ± 3.00	kJ/mol	NIST Webbook
hfs	263.70 ± 2.80	kJ/mol	NIST Webbook
hfs	285.50 ± 2.20	kJ/mol	NIST Webbook

hfus	18.00	kJ/mol	Vapor Pressures and Sublimation Enthalpies of Nickelocene and Cobaltocene Measured by Thermogravimetry
hfus	19.00	kJ/mol	Enthalpies of sublimation of ferrocene and nickelocene measured by calorimetry and the method of Langmuir
hsub	70.20 ± 1.50	kJ/mol	NIST Webbook
hsub	71.50 ± 0.60	kJ/mol	NIST Webbook
hsub	72.40 ± 1.30	kJ/mol	NIST Webbook
ie	6.80 ± 0.10	eV	NIST Webbook
ie	6.75	eV	NIST Webbook
ie	6.51	eV	NIST Webbook
ie	7.20 ± 0.10	eV	NIST Webbook
ie	6.80	eV	NIST Webbook
ie	6.50 ± 0.25	eV	NIST Webbook
ie	6.20	eV	NIST Webbook
ie	6.24	eV	NIST Webbook
ss	253.10	J/mol×K	NIST Webbook
ss	253.00	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	205.40	J/mol×K	298.15	NIST Webbook
cps	171.00	J/mol×K	298.00	NIST Webbook
cps	205.60	J/mol×K	298.15	NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1271289&Units=SI>

Enthalpies of sublimation of ferrocene and nickelocene measured by calorimetry and the method of Langmuir
Vapor Pressures and Sublimation Enthalpies of Nickelocene and Cobaltocene Measured by Thermogravimetry:

<https://www.doi.org/10.1016/j.jct.2011.06.001>

<https://www.doi.org/10.1021/jc200815v>

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
ie:	Ionization energy
ss:	Solid phase molar entropy at standard conditions

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