

Chromium hexacarbonyl

Other names:	Chromcarbonyl Chromium carbonyl Chromium carbonyl (Cr(CO) ₆) Chromium carbonyl (cr(co) ₆), (oc-6-11)- Cr(CO) ₆ Hexacarbonylchromium
Inchi:	InChI=1S/6CO.Cr/c6*1-2;
InchiKey:	KOTQLLUQLXWWDK-UHFFFAOYSA-N
Formula:	C ₆ CrO ₆
SMILES:	[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[Cr]
Mol. weight [g/mol]:	220.06
CAS:	13007-92-6

Physical Properties

Property code	Value	Unit	Source
affp	739.20	kJ/mol	NIST Webbook
basg	714.60	kJ/mol	NIST Webbook
chs	-1949.40 ± 1.80	kJ/mol	NIST Webbook
chs	-1853.90 ± 4.20	kJ/mol	NIST Webbook
chs	-1932.00 ± 17.00	kJ/mol	NIST Webbook
hfs	-932.60 ± 4.80	kJ/mol	NIST Webbook
hfs	-980.40 ± 5.90	kJ/mol	NIST Webbook
hfs	-982.00 ± 2.10	kJ/mol	NIST Webbook
hfs	-978.10 ± 1.40	kJ/mol	NIST Webbook
hfs	-1077.50 ± 4.40	kJ/mol	NIST Webbook
hfs	-980.00 ± 2.00	kJ/mol	NIST Webbook
hfs	-929.20 ± 4.10	kJ/mol	NIST Webbook
hfs	-976.60 ± 5.40	kJ/mol	NIST Webbook
hfs	-999.00 ± 17.00	kJ/mol	NIST Webbook
hsub	69.00 ± 2.00	kJ/mol	NIST Webbook
hsub	72.00 ± 4.20	kJ/mol	NIST Webbook
hsub	70.00 ± 2.00	kJ/mol	NIST Webbook
hsub	69.50	kJ/mol	NIST Webbook
hsub	71.60 ± 1.70	kJ/mol	NIST Webbook
ie	8.14 ± 0.02	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	8.42 ± 0.03	eV	NIST Webbook

ie	8.30 ± 0.05	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.20 ± 0.10	eV	NIST Webbook
ie	8.24 ± 0.07	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.41	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.40 ± 0.02	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.20	eV	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	71.50 ± 0.80	kJ/mol	287.50	NIST Webbook
hsubt	63.30	kJ/mol	328.00	NIST Webbook
hsubt	65.70	kJ/mol	269.00	NIST Webbook
hsubt	68.50 ± 1.10	kJ/mol	357.00	NIST Webbook
hsubt	68.50	kJ/mol	355.50	NIST Webbook
hsubt	71.60 ± 1.70	kJ/mol	260.00	NIST Webbook
hsubt	69.30	kJ/mol	365.00	NIST Webbook
hsubt	63.60	kJ/mol	358.00	NIST Webbook
hvapt	62.50	kJ/mol	366.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.26672e+01
Coeff. B	-7.85221e+03
Coeff. C	7.05000e+00
Temperature range (K), min.	309.15
Temperature range (K), max.	424.15

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C13007926&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
chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
pvap:	Vapor pressure

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