

Benzenechromiumtricarbonyl

Other names:	Chromium, («eta»6-benzene)tricarbonyl- Chromium, (benzene)tricarbonyl- «eta»6-Benzenetricarbonylchromium «pi»-Benzenechromium tricarbonyl «pi»-Benzenetricarbonylchromium (Benzene)tricarbonylchromium Benchrotrene Benzene-chromium carbonyl complex Benzenechromotricarbonyl Benzenetricarbonyl chromium(0) Tricarbonylbenzene chromium Benzentrikarbonylchromium
Inchi:	InChI=1S/C6H6.3CO.Cr/c1-2-4-6-5-3-1;3*1-2;/h1-6H;;;
InchiKey:	WVSBQYMJNMJHIM-UHFFFAOYSA-N
Formula:	C9H6CrO3
SMILES:	[C-]#[O+].[C-]#[O+].[C-]#[O+].[Cr].c1ccccc1
Mol. weight [g/mol]:	214.14
CAS:	12082-08-5

Physical Properties

Property code	Value	Unit	Source
hf	-350.30 ± 9.40	kJ/mol	NIST Webbook
hfs	-441.50 ± 8.40	kJ/mol	NIST Webbook
hsub	91.20 ± 4.20	kJ/mol	NIST Webbook
hsub	91.20	kJ/mol	NIST Webbook
ie	7.28	eV	NIST Webbook
ie	7.30 ± 0.10	eV	NIST Webbook
ie	7.41 ± 0.06	eV	NIST Webbook
ie	7.42 ± 0.03	eV	NIST Webbook
ie	6.70 ± 0.10	eV	NIST Webbook
ie	7.00 ± 0.20	eV	NIST Webbook
ss	267.40	J/molxK	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	238.10	J/mol×K	298.15	NIST Webbook
hsubt	97.90	kJ/mol	367.00	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C12082085&Units=SI>

Legend

cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
ss:	Solid phase molar entropy at standard conditions

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