Ferric tris(acetylacetonate)

Other names:	(Acetylacetonato)iron(iii) (oc-6-11)-tris(2,4-pentanedionato-O,O')-iron Acetope Fe(II) Ferric acetylacetonate Ferric triacetylacetonate Ferric tris(acetoacetonate) Ferric(III) acetylacetonate Iron acetylacetonate Iron triacetylacetonate Iron tris(2,4-pentanedionate) Iron tris(acetoacetonate) Iron tris(acetylacetonate) Iron(3+) acetylacetonate Iron(III) 2,4-pentanedionate Iron(iii) acetylacetonate Iron, tris(2,4-pentanedionato)- NSC 43622 Nacem Iron Tris(2,4-pentanedionato)iron Tris(acetylacetonato)iron Tris(acetylacetone)iron iron, tris(2,4-pentanedionato-O,O')-, (oc-6-11)- tris(pentane-2,4-dionato)iron(II)
Inchi:	InChI=1S/3C5H8O2.Fe/c3*1-4(6)3-5(2)7;/h3*3,6H,1-2H3;/q;;;+3/p-3/b3*4-3-;
InchiKey:	AQBLLJNPHDIAPN-LNTINUHCSA-K
Formula:	C15H21FeO6
SMILES:	CC(=O)C=C(C)[O-].CC(=O)C=C(C)[O-].CC(=O)C=C(C)[O-].[Fe]
Mol. weight [g/mol]:	353.17
CAS:	14024-18-1

Physical Properties

Property code	Value	Unit	Source
ea	1.86 ± 0.02	eV	NIST Webbook
hsub	128.60 ± 0.90	kJ/mol	NIST Webbook
hsub	126.40 ± 3.10	kJ/mol	NIST Webbook
hsub	138.40 ± 5.20	kJ/mol	NIST Webbook

hsub	65.30 ± 3.30	kJ/mol	NIST Webbook
ie	8.45 ± 0.05	eV	NIST Webbook
ie	8.64 ± 0.11	eV	NIST Webbook
ie	7.60 ± 0.20	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	7.89	eV	NIST Webbook
ie	8.10 ± 0.07	eV	NIST Webbook
ss	526.50	J/mol×K	NIST Webbook
tf	461.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	429.90	J/mol×K	298.15	NIST Webbook
hfust	30.10	kJ/mol	459.00	NIST Webbook
hfust	25.30	kJ/mol	460.00	NIST Webbook
hfust	22.60	kJ/mol	462.00	NIST Webbook
hfust	25.90	kJ/mol	454.00	NIST Webbook
hsubt	112.00	kJ/mol	428.00	NIST Webbook
hsubt	124.60 ± 0.90	kJ/mol	378.50	NIST Webbook
hsubt	114.20 ± 1.50	kJ/mol	346.50	NIST Webbook
hsubt	100.00	kJ/mol	395.00	NIST Webbook
hsubt	114.20	kJ/mol	385.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14024181&Units=SI

Effect of the chemical structures of iron complexes on the solubilities in supercritical carbon dioxide: https://www.doi.org/10.1016/j.fluid.2011.05.008

Legend

cps: Solid phase heat capacity

ea: Electron affinity

hfust: Enthalpy of fusion at a given temperature

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
tf:	Normal melting (fusion) point