1,1,1,5,5,5-Hexafluoroacetylacetone iron(III) salt

Other names: Iron, tris(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-O,O')-, (OC-6-11)-
Iron, tris(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato)-
Iron, tris(1,1,1,5,5,5-hexafluoroacetylacetonato)-
Tris(hexafluoroacetylacetonato)iron
Iron, tris(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-O,O'-)
Iron tris(1,1,1,5,5,5-hexafluoroacetylacetate)

Inchi: InChI=1S/3C5H2F6O2.Fe/c3*6-4(7,8)2(12)1-3(13)5(9,10)11;/h3*1,12H;/q;;;+3/p-3/b3*2-1

InchiKey: NBPRJLXRDBDIFS-JVUUZWNBSA-K

Formula: C15H3F18FeO6

SMILES: O=C(C=C([O-])C(F)(F)F)C(F)(F)F.O=C(C=C([O-])C(F)(F)F)C(F)(F)F.O=C(C=C([O-])C(F)(

Mol. weight [g/mol]: 677.00

CAS: 17786-67-3

Physical Properties

Property code	Value	Unit	Source
hsub	79.00 ± 6.50	kJ/mol	NIST Webbook
ie	9.70 ± 0.20	eV	NIST Webbook
ie	9.62 ± 0.05	eV	NIST Webbook
ie	10.20 ± 0.10	eV	NIST Webbook
ie	10.34 ± 0.10	eV	NIST Webbook
ie	10.13 ± 0.07	eV	NIST Webbook
ie	10.14	eV	NIST Webbook
ie	8.28	eV	NIST Webbook
ie	10.13 ± 0.03	eV	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	52.00	kJ/mol	348.00	NIST Webbook
hsubt	60.00	kJ/mol	348.00	NIST Webbook
hsubt	77.60 ± 6.20	kJ/mol	334.00	NIST Webbook
hsubt	109.60 ± 3.80	kJ/mol	335.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17786673&Units=SI

Legend

hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
ie: Ionization energy