

1,1,1,5,5,5-Hexafluoroacetylacetonone 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-hexafluoroacetylacetonato)
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)(F)F)C(F)(F)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

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