

Iron, tricarbonyl[(1,2,3,4-«eta»4)-1,3,5,7-cyclooctatetraene]

Other names:	Cyclooctatetraeneiron tricarbonyl Iron, tricarbonyl[(1,2,3,4-«eta»)-1,3,5,7-cyclooctatetraene]- Iron, tricarbonyl(1,3,5,7-cyclooctatetraene)- Cyclooctatetraenetricarbonyliron Tricarbonyl (1,3,5,7-cyclooctatetraene)iron Tricarbonyl(cyclooctatetraene)iron
Inchi:	InChI=1S/C8H8.3CO.Fe/c1-2-4-6-8-7-5-3-1;3*1-2;/h1-8H;;;;
InchiKey:	XAOCYVWRKJTXOL-UHFFFAOYSA-N
Formula:	C11H8FeO3
SMILES:	C1=CC=CC=C1.[C-]#[O+].[C-]#[O+].[C-]#[O+].[Fe]
Mol. weight [g/mol]:	244.02
CAS:	12093-05-9

Physical Properties

Property code	Value	Unit	Source
hf	-152.00 ± 12.00	kJ/mol	NIST Webbook
hfs	-239.00 ± 11.00	kJ/mol	NIST Webbook
hsub	87.00 ± 4.00	kJ/mol	NIST Webbook
hsub	87.00 ± 4.00	kJ/mol	NIST Webbook
ie	7.80 ± 0.10	eV	NIST Webbook
ie	7.30	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	7.84	eV	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C12093059&Units=SI>

Legend

hf: Enthalpy of formation at standard conditions

hfs: Solid phase enthalpy of formation at standard conditions
hsub: Enthalpy of sublimation at standard conditions
ie: Ionization energy

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