

Iron, (1,3-butadiene)tricarbonyl-

Other names:	Iron, («eta»4-1,3-butadiene)tricarbonyl- (1,3-Butadiene)tricarbonyl iron Butadiene iron tricarbonyl Butadiene tricarbonyl iron Tricarbonyl(1,3-butadiene)iron Tricarbonylbutadiene iron (CH ₂ =CHCH=CH ₂)(CO) ₃ Fe 1,3-Butadiene iron tricarbonyl («eta»4-1,3-Butadiene)tricarbonyliron NSC 58462 («eta»-1,3-butadiene)tricarbonyliron
Inchi:	InChI=1S/C4H6.3CO.Fe/c1-3-4-2;3*1-2;/h3-4H,1-2H2;;;
InchiKey:	NBFCJULAAWWTBL-UHFFFAOYSA-N
Formula:	C ₇ H ₆ FeO ₃
SMILES:	C=CC=C.[C-]#[O+].[C-]#[O+].[C-]#[O+].[Fe]
Mol. weight [g/mol]:	193.97
CAS:	12078-32-9

Physical Properties

Property code	Value	Unit	Source
ea	0.90	eV	NIST Webbook
hf	-358.80 ± 7.10	kJ/mol	NIST Webbook
hfl	-407.80 ± 5.70	kJ/mol	NIST Webbook
hvap	49.00 ± 4.20	kJ/mol	NIST Webbook
ie	8.22	eV	NIST Webbook
ie	8.16	eV	NIST Webbook
ie	8.23	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
ie	8.04	eV	NIST Webbook
ie	8.16	eV	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C12078329&Units=SI>

Legend

ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy

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