# Iron, (1,3-butadiene)tricarbonyl-

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|---|---|
| **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 |
| | (CH2=CHCH=CH2)(CO)3Fe |
| | 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:** | C7H6FeO3 |
| **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 |