Ferrocene, benzoyl-

Other names:	Benzoyl ferrocene
	Benzoyldicyclopentadienyliron
	Ferrecenophenone
	Ferrocenyl phenyl ketone
	Iron(II), (benzoylcyclopentadienyl)cyclopentadienyl-
	Ketone, ferrocenyl phenyl
	Methanone, ferrocenylphenyl-
	Monobenzoylferrocene
	NSC 54800
	benzoylferrocene
Inchi:	InChI=1S/C12H9O.C5H5.Fe/c13-12(11-8-4-5-9-11)10-6-2-1-3-7-10;1-2-4-5-3-1;/h1-9H;1-
InchiKey:	JJHHJZCYDPLHIL-UHFFFAOYSA-N
Formula:	C17H14FeO
SMILES:	O=C(c1ccccc1)C12C3C4C5C1[Fe]45321678C2C1C6C7C28
Mol. weight [g/mol]:	290.14
CAS:	1272-44-2

Physical Properties

Property code	Value	Unit	Source
hfus	29.90	kJ/mol	Vapour pressures and enthalpies of vaporization of a series of the ferrocene derivatives
hfus	29.90	kJ/mol	The heat capacities and thermodynamic functions of some derivatives of ferrocene
hsub	116.00 ± 6.00	kJ/mol	NIST Webbook
hsub	119.90 ± 0.70	kJ/mol	NIST Webbook
hsub	116.30 ± 6.00	kJ/mol	NIST Webbook
hvap	98.20 ± 0.30	kJ/mol	NIST Webbook
pc	1590.00	kPa	Critical point measurement of ferrocene and some of its derivatives
tf	384.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	387.90	J/mol×K	298.00	NIST Webbook
hfust	29.90	kJ/mol	189.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1272442&Units=SI
Critical point measurement of ferrocene and some of its derivatives:	https://www.doi.org/10.1016/j.fluid.2012.03.021
Vapour pressures and enthalpies of vaporization of a series of the ferrocene derivatives:	https://www.doi.org/10.1016/j.jct.2006.09.001
The heat capacities and thermodynamic functions of some derivatives of ferrocene:	https://www.doi.org/10.1016/j.jct.2007.12.003

Legend

cps:	Solid phase heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
pc:	Critical Pressure
tf:	Normal melting (fusion) point