

Bis(cyclopentadienyl)zirconium dichloride

Other names:	Bis(cyclopentadienyl)dichlorozirconium Bis-«pi»-cyclopentadienyldichlorozirconium Bis-Â«piÂ»-cyclopentadienyldichlorozirconium Dichlorobis(cyclopentadienyl) zirconium Dichlorobis(«eta»5-2,4-cyclopentadien-1-yl)zirconium Dichlorobis(Â«etaÂ»5-2,4-cyclopentadien-1-yl)zirconium Dichlorodi-«pi»-cyclopentadienylzirconium Dichlorodi-«pi»-dicyclopentadienylzirconium Dichlorodi-Â«piÂ»-cyclopentadienylzirconium Dichlorodi-Â«piÂ»-dicyclopentadienylzirconium Dichlorodicyclopentadienylzirconium Dichlorozirconocene Dicyclopentadienyldichlorozirconium Dicyclopentadienylzirconium dichloride NSC 93930 Zirconcene dichloride Zirconium dicyclopentadiene dichloride Zirconium, dichlorobis(2,4-cyclopentadien-1-yl)- Zirconium, dichlorobis(«eta»(5)-2,4-cyclopentadien-1-yl)- Zirconium, dichlorobis(Â«etaÂ»(5)-2,4-cyclopentadien-1-yl)- Zirconium, dichlorodi-«pi»-cyclopentadienyl- Zirconium, dichlorodi-Â«piÂ»-cyclopentadienyl- Zirconocene dichloride bis(3-cyclopentadienyl)dichlorozirconium bis(eta-cyclopentadienyl)zirconium chloride
Inchi:	InChI=1S/2C5H5.2ClH.Zr/c2*1-2-4-5-3-1;;;/h2*1-5H;2*1H;/q;;;+2/p-2
InchiKey:	QRUYYSPOGSGZGQ-UHFFFAOYSA-L
Formula:	C10H10Cl2Zr
SMILES:	Cl[Zr]12345678(Cl)(C9C1C2C3C94)C1C5C6C7C18
Mol. weight [g/mol]:	292.32
CAS:	1291-32-3

Physical Properties

Property code	Value	Unit	Source
chs	-5972.70 ± 2.90	kJ/mol	NIST Webbook
hf	-433.60 ± 3.90	kJ/mol	NIST Webbook

hfs	-538.60 ± 3.30		kJ/mol	NIST Webbook
hsub	103.00 ± 13.00		kJ/mol	NIST Webbook
hsub	108.50 ± 4.60		kJ/mol	NIST Webbook
hsub	105.00 ± 2.10		kJ/mol	NIST Webbook
hsub	81.20 ± 2.10		kJ/mol	NIST Webbook
hsub	105.00 ± 2.10		kJ/mol	NIST Webbook
ie	9.37 ± 0.25		eV	NIST Webbook
ie	8.60 ± 0.10		eV	NIST Webbook
ie	8.60 ± 0.05		eV	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	100.30	kJ/mol	425.00	NIST Webbook
hvapt	71.00 ± 5.00	kJ/mol	409.50	NIST Webbook
pvap	9.20e-05	kPa	408.15	Vapor pressure of tetrakis(1,1,1-trifluoro-5,6-dimethylheptanedionato) zirconium(IV) and dichlorobis(5-cyclopentadienyl)zirconium(IV) by TG-based transpiration technique
pvap	1.69e-04	kPa	418.15	Vapor pressure of tetrakis(1,1,1-trifluoro-5,6-dimethylheptanedionato) zirconium(IV) and dichlorobis(5-cyclopentadienyl)zirconium(IV) by TG-based transpiration technique
pvap	3.11e-04	kPa	429.15	Vapor pressure of tetrakis(1,1,1-trifluoro-5,6-dimethylheptanedionato) zirconium(IV) and dichlorobis(5-cyclopentadienyl)zirconium(IV) by TG-based transpiration technique
pvap	5.47e-04	kPa	438.15	Vapor pressure of tetrakis(1,1,1-trifluoro-5,6-dimethylheptanedionato) zirconium(IV) and dichlorobis(5-cyclopentadienyl)zirconium(IV) by TG-based transpiration technique

pvap	9.14e-04	kPa	449.15	Vapor pressure of tetrakis(1,1,1-trifluoro-5,6-dimethylheptanedionato)zirconium(IV) and dichlorobis(5-cyclopentadienyl)zirconium(IV) by TG-based transpiration technique
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Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.39147e+01
Coeff. B	-1.20678e+04
Temperature range (K), min.	510.76
Temperature range (K), max.	648.70

Sources

Vapor pressure of tetrakis(1,1,1-trifluoro-5,6-dimethylheptanedionato)zirconium(IV) and dichlorobis(5-cyclopentadienyl)zirconium(IV) by TG-based transpiration technique: Pressure: <https://www.doi.org/10.1016/j.tca.2008.08.010>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1291323&Units=SI>
<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Legend

chs: Standard solid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
pvap: Vapor pressure

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