

Dirhenium decacarbonyl

Other names:	Re2(CO)10 Rhenium carbonyl Rhenium carbonyl (Re2(CO)10) Rhenium, decacarbonyldi-, Rhenium, decacarbonyldi-, (Re-Re) decacarbonyldirhenium
Inchi:	InChI=1S/10CO.2Re/c10*1-2;;
InchiKey:	ZIZHEHXAMPQGEK-UHFFFAOYSA-N
Formula:	C10O10Re2
SMILES:	[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].
Mol. weight [g/mol]:	652.51
CAS:	14285-68-8

Physical Properties

Property code	Value	Unit	Source
chs	-3589.50 ± 2.50	kJ/mol	NIST Webbook
hf	-1544.10 ± 6.40	kJ/mol	NIST Webbook
hf	-1556.70 ± 3.90	kJ/mol	NIST Webbook
hf	-1557.10 ± 9.10	kJ/mol	NIST Webbook
hf	-1554.40 ± 7.30	kJ/mol	NIST Webbook
hf	-1560.00 ± 14.00	kJ/mol	NIST Webbook
hfs	-1658.00 ± 8.90	kJ/mol	NIST Webbook
hfs	-1661.00 ± 14.00	kJ/mol	NIST Webbook
hfs	-1657.60 ± 3.40	kJ/mol	NIST Webbook
hfs	-1645.00 ± 6.10	kJ/mol	NIST Webbook
hfs	-1655.30 ± 7.00	kJ/mol	NIST Webbook
hsub	101.00 ± 2.00	kJ/mol	NIST Webbook
hsub	101.00 ± 2.00	kJ/mol	NIST Webbook
hsub	93.30 ± 4.20	kJ/mol	NIST Webbook
ie	8.07	eV	NIST Webbook
ie	8.36 ± 0.03	eV	NIST Webbook
ie	8.49 ± 0.02	eV	NIST Webbook
ie	8.86	eV	NIST Webbook

tt

366.75

K

A force field for MD simulations on rhenium organometallic compounds developed from enthalpy of sublimation and X-ray diffraction measurements

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	77.60	kJ/mol	406.50	NIST Webbook
hvapt	68.70	kJ/mol	468.50	NIST Webbook

Sources

A force field for MD simulations on rhenium organometallic compounds developed from enthalpy of sublimation and X-ray diffraction measurements:

<https://www.doi.org/10.1016/j.jct.2019.01.016>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C14285688&Units=SI>

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
tt:	Triple Point Temperature

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