

# Dirhenium decacarbonyl

<b>Other names:</b>	Re <sub>2</sub> (CO) <sub>10</sub> Rhenium carbonyl Rhenium carbonyl (Re <sub>2</sub> (CO) <sub>10</sub> ) Rhenium, decacarbonyldi-, Rhenium, decacarbonyldi-, (Re-Re) decacarbonyldirhenium
<b>Inchi:</b>	InChI=1S/10CO.2Re/c10*1-2;;
<b>InchiKey:</b>	ZIZHEHXAMPQGEK-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>10</sub> O <sub>10</sub> Re <sub>2</sub>
<b>SMILES:</b>	[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].
<b>Mol. weight [g/mol]:</b>	652.51
<b>CAS:</b>	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	-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
hf	-1556.70 ± 3.90	kJ/mol	NIST Webbook
hfs	-1655.30 ± 7.00	kJ/mol	NIST Webbook
hfs	-1645.00 ± 6.10	kJ/mol	NIST Webbook
hfs	-1657.60 ± 3.40	kJ/mol	NIST Webbook
hfs	-1661.00 ± 14.00	kJ/mol	NIST Webbook
hfs	-1658.00 ± 8.90	kJ/mol	NIST Webbook
hsub	101.00 ± 2.00	kJ/mol	NIST Webbook
hsub	93.30 ± 4.20	kJ/mol	NIST Webbook
hsub	101.00 ± 2.00	kJ/mol	NIST Webbook
ie	8.36 ± 0.03	eV	NIST Webbook
ie	8.07	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
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## 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

<b>chs:</b>	Standard solid enthalpy of combustion
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>tt:</b>	Triple Point Temperature

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