9H-Fluoren-9-one

Other names:	9(9H)-fluorenone
	9-fluorenone
	9H-Fluorene-9-one
	Fluoren-9-one
	Fluorenone
Inchi:	InChI=1S/C13H8O/c14-13-11-7-3-1-5-9(11)10-6-2-4-8-12(10)13/h1-8H
InchiKey:	YLQWCDOCJODRMT-UHFFFAOYSA-N
Formula:	C13H8O
SMILES:	O=C1c2ccccc2-c2ccccc21
Mol. weight [g/mol]:	180.20
CAS:	486-25-9

Physical Properties

Property code	Value	Unit	Source
chs	-6222.80 ± 2.10	kJ/mol	NIST Webbook
gf	234.21	kJ/mol	Joback Method
hf	52.30 ± 2.30	kJ/mol	NIST Webbook
hfs	-36.10 ± 2.30	kJ/mol	NIST Webbook
hfus	16.36	kJ/mol	Thermodynamic properties of 9-fluorenone: Mutual validation of experimental and computational results
hfus	17.60	kJ/mol	Experimental and Computational Study of the Thermodynamic Properties of 9-Fluorenone and 9-Fluorenol
hsub	88.40 ± 0.40	kJ/mol	NIST Webbook
hsub	93.90 ± 1.80	kJ/mol	NIST Webbook
hsub	88.40 ± 0.40	kJ/mol	NIST Webbook
hsub	88.40	kJ/mol	NIST Webbook
hvap	54.53	kJ/mol	Joback Method
ie	8.36 ± 0.03	eV	NIST Webbook
ie	8.29	eV	NIST Webbook
ie	8.36 ± 0.02	eV	NIST Webbook
log10ws	-4.28		Crippen Method
logp	2.898		Crippen Method
mcvol	137.220	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method

rinpol	1705.00		NIST Webbook
rinpol	293.70		NIST Webbook
rinpol	294.30		NIST Webbook
rinpol	294.49		NIST Webbook
rinpol	293.88		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	294.79		NIST Webbook
rinpol	294.50		NIST Webbook
rinpol	293.70		NIST Webbook
rinpol	290.24		NIST Webbook
rinpol	293.09		NIST Webbook
rinpol	291.28		NIST Webbook
rinpol	293.60		NIST Webbook
rinpol	294.13		NIST Webbook
rinpol	294.79		NIST Webbook
rinpol	293.60		NIST Webbook
rinpol	294.30		NIST Webbook
rinpol	294.49		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	294.03		NIST Webbook
rinpol	294.30		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	293.64		NIST Webbook
rinpol	292.60		NIST Webbook
rinpol	1752.00		NIST Webbook
ripol	2697.00		NIST Webbook
ripol	2697.00		NIST Webbook
tb	614.70	K	NIST Webbook
tc	892.23	K	Joback Method
tf	357.15 ± 2.00	K	NIST Webbook
tf	355.00 ± 4.00	K	NIST Webbook
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	395.47	J/mol×K	892.23	Joback Method
cpg	342.59	J/mol×K	674.41	Joback Method
cpg	354.95	J/mol×K	717.98	Joback Method
cpg	366.32	J/mol×K	761.54	Joback Method
cpg	376.79	J/mol×K	805.11	Joback Method
cpg	386.47	J/mol×K	848.67	Joback Method
cpg	329.11	J/mol×K	630.85	Joback Method
hfust	18.12	kJ/mol	356.40	NIST Webbook
hfust	18.12	kJ/mol	356.40	NIST Webbook
hfust	14.85	kJ/mol	353.30	NIST Webbook
hsubt	87.60 ± 0.30	kJ/mol	319.00	NIST Webbook
hvapt	60.90	kJ/mol	435.00	NIST Webbook
hvapt	59.80	kJ/mol	475.00	NIST Webbook
hvapt	59.10	kJ/mol	525.00	NIST Webbook
hvapt	58.60	kJ/mol	565.00	NIST Webbook
hvapt	57.90	kJ/mol	595.00	NIST Webbook
psub	5.99e-04	kPa	337.90	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	5.40e-04	kPa	336.60	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	5.96e-04	kPa	337.80	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique

psub	5.28e-04	kPa	336.50	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	9.37e-04	kPa	342.70	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	9.52e-04	kPa	342.80	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	3.45e-04	kPa	331.90	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	3.19e-04	kPa	331.10	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	

psub	3.11e-04	kPa	330.90	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	2.45e-04	kPa	328.60	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	2.46e-04	kPa	328.40	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	1.67e-04	kPa	324.70	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	1.59e-04	kPa	324.50	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	

psub	1.43e-04	kPa	323.10	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	1.39e-04	kPa	323.00	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	6.16e-05	kPa	315.10	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	5.09e-05	kPa	313.10	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	5.10e-05	kPa	313.00	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	

psub	3.65e-05	kPa	309.80	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	2.79e-05	kPa	307.90	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	1.69e-05	kPa	303.60	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	1.21e-05	kPa	300.80	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solid Liquid Phase Equilibrium and Solubility of Dibenzo[b,d]furan and 9H-Fluoren-9-One in Organic Solvents:	https://www.doi.org/10.1021/je201282d
Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique:	https://www.doi.org/10.1016/j.jct.2010.01.014
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C486259&Units=SI
Thermodynamic properties of 9-fluorenone: Mutual validation of experimental and computational results:	https://www.doi.org/10.1016/j.jct.2012.05.003
Joback Method	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and Computational Study of the Thermodynamic Properties of 9-Fluorenone and 9-Fluorenol :	https://www.doi.org/10.1021/je300584m

Solid-liquid phase equilibrium of 9-fluorenone and several polynuclear aromatic hydrocarbons:	https://www.doi.org/10.1016/j.fluid.2012.01.017
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of 9-fluorenone, thianthrene and xanthene in organic solvents:	https://www.doi.org/10.1016/j.fluid.2005.02.016

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume