Phenanthrene, 9,10-dihydro-

Other names: 9,10-Dihydrophenanthrene
Inchi: InChI=1S/C14H12/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h1-8H,9-10H2
InchiKey: XXPBFNVKTVJZKF-UHFFFAOYSA-N
Formula: C14H12
SMILES: c1ccc2c(c1)CCc1ccccc1-2
Mol. weight [g/mol]: 180.25
CAS: 776-35-2

Physical Properties

Property code	Value	Unit	Source
chs	-7290.40 ± 1.00	kJ/mol	NIST Webbook
gf	353.12	kJ/mol	Joback Method
hf	154.60 ± 1.60	kJ/mol	NIST Webbook
hf	155.10 ± 1.60	kJ/mol	NIST Webbook
hfs	66.30 ± 1.20	kJ/mol	NIST Webbook
hfus	18.48	kJ/mol	Joback Method
hsub	88.80	kJ/mol	NIST Webbook
hvap	76.60 ± 0.10	kJ/mol	NIST Webbook
ie	7.55 ± 0.02	eV	NIST Webbook
ie	8.08 ± 0.06	eV	NIST Webbook
ie	8.19	eV	NIST Webbook
log10ws	-4.74		Crippen Method
logp	3.452		Crippen Method
mcvol	149.740	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
rinpol	1685.40		NIST Webbook
rinpol	1688.60		NIST Webbook
rinpol	1673.50		NIST Webbook
rinpol	1689.80		NIST Webbook
rinpol	1699.50		NIST Webbook
rinpol	1689.30		NIST Webbook
rinpol	1700.30		NIST Webbook
rinpol	1673.50		NIST Webbook
rinpol	1689.80		NIST Webbook
rinpol	1699.50		NIST Webbook
rinpol	1689.30		NIST Webbook
rinpol	1668.00		NIST Webbook

rinpol	1697.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	286.80		NIST Webbook
rinpol	287.00		NIST Webbook
rinpol	287.33		NIST Webbook
rinpol	286.40		NIST Webbook
rinpol	287.09		NIST Webbook
rinpol	288.60		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	286.22		NIST Webbook
rinpol	287.09		NIST Webbook
rinpol	1697.00		NIST Webbook
rinpol	286.80		NIST Webbook
rinpol	287.86		NIST Webbook
rinpol	1688.60		NIST Webbook
ss	229.29	J/mol×K	NIST Webbook
ss	229.40	J/mol×K	NIST Webbook
tb	590.18	K	Joback Method
tc	841.42	K	Joback Method
tf	370.00 ± 1.00	K	NIST Webbook
tf	370.00 ± 1.00	K	NIST Webbook
tf	308.00 ± 3.00	K	NIST Webbook
tt	306.52 ± 0.02	K	NIST Webbook
tt	306.52 ± 0.00	K	NIST Webbook
tt	306.51 ± 0.01	K	NIST Webbook
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.58	J/mol×K	673.93	Joback Method
cpg	370.70	J/mol×K	632.05	Joback Method
cpg	434.09	J/mol×K	841.42	Joback Method
cpg	423.34	J/mol×K	799.55	Joback Method
cpg	411.76	J/mol×K	757.67	Joback Method
cpg	399.22	J/mol×K	715.80	Joback Method
cpg	354.45	J/mol×K	590.18	Joback Method
cps	243.08	J/mol×K	298.15	NIST Webbook
cps	243.80	J/mol×K	298.15	NIST Webbook
dvisc	0.0011961	Pa×s	390.96	Joback Method
dvisc	0.0009195	Pa×s	430.81	Joback Method

dvisc	0.0007391	Pa×s	470.65	Joback Method
dvisc	0.0006147	Pa×s	510.49	Joback Method
dvisc	0.0005250	Pa×s	550.34	Joback Method
dvisc	0.0016514	Pa×s	351.12	Joback Method
dvisc	0.0004581	Pa×s	590.18	Joback Method
hfust	12.80	kJ/mol	306.50	NIST Webbook
hfust	12.80	kJ/mol	306.50	NIST Webbook
hfust	12.79	kJ/mol	306.52	NIST Webbook
hvapt	72.30 ± 0.60	kJ/mol	385.50	NIST Webbook
hvapt	64.00	kJ/mol	435.00	NIST Webbook
sfust	41.73	J/mol×K	306.52	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	441.70	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.52938e+01
Coeff. B	-1.07767e+04
Temperature range (K), min.	430.96
Temperature range (K), max.	539.31

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C776352&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
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
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume