Anthracene, 1,2,3,4,5,6,7,8-octahydro-

Other names:	1,2,3,4,5,6,7,8-Octahydroanthracene
	Anthracene, octahydro-
	Octahydroanthracene
	s-Octahydroanthracene
	sym-Octahydroanthracene
Inchi:	InChI=1S/C14H18/c1-2-6-12-10-14-8-4-3-7-13(14)9-11(12)5-1/h9-10H,1-8H2
InchiKey:	LFAYMJXHGYUQNV-UHFFFAOYSA-N
Formula:	C14H18
SMILES:	c1c2c(cc3c1CCCC3)CCCC2
Mol. weight [g/mol]:	186.29
CAS:	1079-71-6

Physical Properties

Property code	Value	Unit	Source
affp	845.40	kJ/mol	NIST Webbook
basg	814.70	kJ/mol	NIST Webbook
chs	-7962.10 ± 2.90	kJ/mol	NIST Webbook
gf	263.24	kJ/mol	Joback Method
hf	-37.20 ± 3.20	kJ/mol	NIST Webbook
hfs	-119.50 ± 2.90	kJ/mol	NIST Webbook
hfus	14.82	kJ/mol	Joback Method
hsub	82.30 ± 1.20	kJ/mol	NIST Webbook
hsub	82.00 ± 1.00	kJ/mol	NIST Webbook
hsub	82.30	kJ/mol	NIST Webbook
hvap	51.81	kJ/mol	Joback Method
ie	7.86 ± 0.05	eV	NIST Webbook
log10ws	-4.47		Crippen Method
logp	3.444		Crippen Method
mcvol	162.640	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	1703.20		NIST Webbook
rinpol	286.84		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	287.69		NIST Webbook
rinpol	287.69		NIST Webbook
rinpol	287.07		NIST Webbook
rinpol	287.07		NIST Webbook

rinpol	1645.00		NIST Webbook
rinpol	286.84		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1694.10		NIST Webbook
rinpol	1694.10		NIST Webbook
rinpol	1680.20		NIST Webbook
rinpol	1694.10		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1680.20		NIST Webbook
rinpol	1694.10		NIST Webbook
rinpol	1703.20		NIST Webbook
rinpol	1694.10		NIST Webbook
rinpol	1694.10		NIST Webbook
rinpol	1684.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1704.00		NIST Webbook
ripol	2153.00		NIST Webbook
tb	567.20	K	NIST Webbook
tc	836.40	K	Joback Method
tf	347.00 ± 6.00	K	NIST Webbook
tf	346.00 ± 1.00	K	NIST Webbook
tf	347.00 ± 6.00	K	NIST Webbook
tf	346.15 ± 1.50	K	NIST Webbook
tf	346.40 ± 1.00	K	NIST Webbook
tt	345.39 ± 0.01	K	NIST Webbook
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.95	J/mol×K	836.40	Joback Method
cpg	471.46	J/mol×K	714.55	Joback Method
cpg	454.28	J/mol×K	673.93	Joback Method
cpg	435.72	J/mol×K	633.32	Joback Method
cpg	415.67	J/mol×K	592.70	Joback Method
cpg	502.17	J/mol×K	795.78	Joback Method
cpg	487.38	J/mol×K	755.17	Joback Method
cps	327.60	J/mol×K	327.00	NIST Webbook
dvisc	0.0022319	Pa×s	348.84	Joback Method
dvisc	0.0010461	Pa×s	430.13	Joback Method
dvisc	0.0007900	Pa×s	470.77	Joback Method

dvisc	0.0006239	Pa×s	511.41	Joback Method
dvisc	0.0005101	Pa×s	552.06	Joback Method
dvisc	0.0014688	Pa×s	389.48	Joback Method
dvisc	0.0004287	Pa×s	592.70	Joback Method
hfust	18.34	kJ/mol	345.40	NIST Webbook
hfust	2.51	kJ/mol	331.40	NIST Webbook
hfust	17.91	kJ/mol	346.00	NIST Webbook
hfust	18.34	kJ/mol	345.40	NIST Webbook
hvapt	45.60	kJ/mol	467.50	NIST Webbook
sfust	53.10	J/mol×K	345.40	NIST Webbook
sfust	7.59	J/mol×K	331.40	NIST Webbook
sfust	51.80	J/mol×K	346.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	440.20	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.18648e+01
Coeff. B	-8.51461e+03
Coeff. C	-3.52500e+01
Temperature range (K), min.	429.86
Temperature range (K), max.	549.63

Sources

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1079716&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
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