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

Other names:	1,2,3,4,5,6,7,8-0ctahydrophenanthrene
	1,2,3,4,5,6,7,8-Octahydrophenanthrene
	Octahydrophenanthrene
	Octahydrophenanthrene, symm.
Inchi:	InChI=1S/C14H18/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h9-10H,1-8H2
InchiKey:	YSZLFGZFQTTZIQ-UHFFFAOYSA-N
Formula:	C14H18
SMILES:	c1cc2c(c3c1CCCC3)CCCC2
Mol. weight [g/mol]:	186.29
CAS:	5325-97-3

Physical Properties

Property code	Value	Unit	Source
affp	846.20	kJ/mol	NIST Webbook
affp	838.90	kJ/mol	NIST Webbook
basg	812.10	kJ/mol	NIST Webbook
basg	815.50	kJ/mol	NIST Webbook
gf	263.24	kJ/mol	Joback Method
hf	43.79	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	51.81	kJ/mol	Joback Method
ie	7.89 ± 0.05	eV	NIST Webbook
ie	8.79 ± 0.02	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	1721.10		NIST Webbook
rinpol	1705.50		NIST Webbook
rinpol	1721.10		NIST Webbook
rinpol	1730.60		NIST Webbook
rinpol	1705.50		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1730.60		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1696.00		NIST Webbook

rinpol	292.30		NIST Webbook
rinpol	291.63		NIST Webbook
rinpol	292.03		NIST Webbook
rinpol	291.40		NIST Webbook
rinpol	292.03		NIST Webbook
rinpol	292.30		NIST Webbook
rinpol	1696.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1694.00		NIST Webbook
rinpol	1716.00		NIST Webbook
tb	568.20	K	NIST Webbook
tc	836.40	K	Joback Method
tf	348.84	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.67	J/mol×K	592.70	Joback Method
cpg	435.72	J/mol×K	633.32	Joback Method
cpg	454.28	J/mol×K	673.93	Joback Method
cpg	471.46	J/mol×K	714.55	Joback Method
cpg	487.38	J/mol×K	755.17	Joback Method
cpg	502.17	J/mol×K	795.78	Joback Method
cpg	515.95	J/mol×K	836.40	Joback Method
dvisc	0.0022319	Pa×s	348.84	Joback Method
dvisc	0.0014688	Pa×s	389.48	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	0.0004287	Pa×s	592.70	Joback Method
hvapt	55.80	kJ/mol	486.00	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.39396e+01
Coeff. B	-1.00510e+04
Coeff. C	-8.75000e+00
Temperature range (K), min.	433.70
Temperature range (K), max.	548.31

Sources

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=C5325973&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

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume