Phenanthrene, 4-methyl-

Other names: 4-Methylphenanthrene
Inchi: InChI=1S/C15H12/c1-11-5-4-7-13-10-9-12-6-2-3-8-14(12)15(11)13/h2-10H,1H3
InchiKey: LOCGAKKLRVLQAM-UHFFFAOYSA-N
Formula: C15H12
SMILES: Cc1cccc2ccc3ccccc3c12
Mol. weight [g/mol]: 192.26
CAS: 832-64-4

Physical Properties

Property code	Value	Unit	Source
chs	-7720.05 ± 0.56	kJ/mol	NIST Webbook
gf	381.87	kJ/mol	Joback Method
hf	195.80 ± 1.10	kJ/mol	NIST Webbook
hfs	102.42 ± 0.67	kJ/mol	NIST Webbook
hfus	21.91	kJ/mol	Joback Method
hsub	93.40	kJ/mol	NIST Webbook
hvap	55.86	kJ/mol	Joback Method
ie	7.70 ± 0.02	eV	NIST Webbook
ie	7.70 ± 0.02	eV	NIST Webbook
ie	7.10 ± 0.10	eV	NIST Webbook
log10ws	-5.56		Crippen Method
logp	4.301		Crippen Method
mcvol	159.530	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	323.30		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	322.92		NIST Webbook
rinpol	322.78		NIST Webbook
rinpol	322.87		NIST Webbook
rinpol	323.28		NIST Webbook
rinpol	323.24		NIST Webbook
rinpol	322.90		NIST Webbook
rinpol	323.10		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	322.81		NIST Webbook
rinpol	323.17		NIST Webbook
rinpol	322.74		NIST Webbook

rinpol	322.74		NIST Webbook
rinpol	322.78		NIST Webbook
rinpol	322.90		NIST Webbook
rinpol	322.80		NIST Webbook
rinpol	321.82		NIST Webbook
rinpol	323.10		NIST Webbook
rinpol	322.80		NIST Webbook
rinpol	323.30		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	322.92		NIST Webbook
rinpol	322.90		NIST Webbook
rinpol	323.17		NIST Webbook
ss	244.55	J/mol×K	NIST Webbook
ss	244.55	J/mol×K	NIST Webbook
tb	617.20	K	Joback Method
tc	866.35	K	Joback Method
tf	375.67	K	Joback Method
tt	324.92 ± 0.01	K	NIST Webbook
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.22	J/mol×K	617.20	Joback Method
cpg	410.54	J/mol×K	700.25	Joback Method
cpg	396.50	J/mol×K	658.73	Joback Method
cpg	456.90	J/mol×K	866.35	Joback Method
cpg	446.52	J/mol×K	824.83	Joback Method
cpg	435.41	J/mol×K	783.30	Joback Method
cpg	423.46	J/mol×K	741.78	Joback Method
cps	263.13	J/mol×K	298.15	NIST Webbook
cps	263.13	J/mol×K	298.15	NIST Webbook
dvisc	0.0010334	Pa×s	415.93	Joback Method
dvisc	0.0008255	Pa×s	456.18	Joback Method
dvisc	0.0006839	Pa×s	496.44	Joback Method
dvisc	0.0005828	Pa×s	536.69	Joback Method
dvisc	0.0005079	Pa×s	576.95	Joback Method
dvisc	0.0004506	Pa×s	617.20	Joback Method
dvisc	0.0013574	Pa×s	375.67	Joback Method
hfust	14.04	kJ/mol	324.90	NIST Webbook
hfust	0.02	kJ/mol	182.00	NIST Webbook

hfust	0.03	kJ/mol	295.00	NIST Webbook
hfust	14.04	kJ/mol	324.90	NIST Webbook
hvapt	69.20 ± 0.10	kJ/mol	507.50	NIST Webbook
hvapt	71.80 ± 0.10	kJ/mol	507.50	NIST Webbook
hvapt	74.40 ± 0.20	kJ/mol	507.50	NIST Webbook
hvapt	61.60 ± 0.10	kJ/mol	507.50	NIST Webbook
hvapt	64.20 ± 0.10	kJ/mol	507.50	NIST Webbook
hvapt	66.70 ± 0.10	kJ/mol	507.50	NIST Webbook
sfust	43.21	J/mol×K	324.90	NIST Webbook
sfust	0.11	J/mol×K	295.00	NIST Webbook
sfust	0.12	J/mol×K	182.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37620e+01
Coeff. B	-4.67696e+03
Coeff. C	-1.14900e+02
Temperature range (K), min.	462.00
Temperature range (K), max.	668.35

Sources

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=C832644&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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume