Anthracene, 1-methyl-

Other names:	1-Methylanthracene
	4-Methylanthracene
Inchi:	InChI=1S/C15H12/c1-11-5-4-8-14-9-12-6-2-3-7-13(12)10-15(11)14/h2-10H,1H3
InchiKey:	KZNJSFHJUQDYHE-UHFFFAOYSA-N
Formula:	C15H12
SMILES:	Cc1cccc2cc3ccccc3cc12
Mol. weight [g/mol]:	192.26
CAS:	610-48-0

Physical Properties

Property code	Value	Unit	Source
ea	0.52 ± 0.02	eV	NIST Webbook
ea	0.55 ± 0.10	eV	NIST Webbook
gf	381.87	kJ/mol	Joback Method
hf	242.80	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	87.00 ± 1.00	kJ/mol	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	1966.00		NIST Webbook
rinpol	322.60		NIST Webbook
rinpol	343.34		NIST Webbook
rinpol	323.33		NIST Webbook
rinpol	1934.80		NIST Webbook
rinpol	1959.30		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	315.90		NIST Webbook
rinpol	323.30		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	323.30		NIST Webbook
rinpol	1934.80		NIST Webbook
rinpol	1959.30		NIST Webbook
rinpol	1976.30		NIST Webbook
rinpol	1920.70		NIST Webbook
rinpol	1934.80		NIST Webbook

rinpol	1959.30		NIST Webbook
rinpol	1976.30		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	315.90		NIST Webbook
rinpol	316.00		NIST Webbook
rinpol	323.33		NIST Webbook
rinpol	323.38		NIST Webbook
rinpol	322.20		NIST Webbook
rinpol	323.30		NIST Webbook
rinpol	327.70		NIST Webbook
rinpol	323.33		NIST Webbook
tb	636.20	K	NIST Webbook
tc	866.35	K	Joback Method
tf	375.67	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.90	J/mol×K	866.35	Joback Method
cpg	396.50	J/mol×K	658.73	Joback Method
cpg	410.54	J/mol×K	700.25	Joback Method
cpg	423.46	J/mol×K	741.78	Joback Method
cpg	435.41	J/mol×K	783.30	Joback Method
cpg	446.52	J/mol×K	824.83	Joback Method
cpg	381.22	J/mol×K	617.20	Joback Method
dvisc	0.0013574	Pa×s	375.67	Joback Method
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
pvap	1.59	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.48	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.74	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.09	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.31	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.25	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.13	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.28	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	5.75	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.19	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.12	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.07	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.04	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.02	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.01	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	5.05e-03	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.34e-03	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.02e-03	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.19e-04	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.60e-04	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	5.68e-05	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.85e-05	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.49e-05	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.27019e+01
Coeff. B	-4.20009e+03
Coeff. C	-1.16618e+02
Temperature range (K), min.	454.94
Temperature range (K), max.	684.93

Sources

Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:	https://www.doi.org/10.1021/je800300x
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=C610480&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

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
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