Anthracene, 2-methyl-

Other names: 2-Methylanthracene
Inchi: InChI=1S/C15H12/c1-11-6-7-14-9-12-4-2-3-5-13(12)10-15(14)8-11/h2-10H,1H3
InchiKey: GYMFBYTZOGMSQJ-UHFFFAOYSA-N
Formula: C15H12
SMILES: Cc1ccc2cc3ccccc3cc2c1
Mol. weight [g/mol]: 192.26
CAS: 613-12-7

Physical Properties

Property code	Value	Unit	Source
affp	884.90	kJ/mol	NIST Webbook
affp	887.50	kJ/mol	NIST Webbook
basg	857.70	kJ/mol	NIST Webbook
basg	855.10	kJ/mol	NIST Webbook
gf	381.87	kJ/mol	Joback Method
hf	242.80	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	84.40 ± 1.20	kJ/mol	NIST Webbook
hvap	84.50 ± 2.70	kJ/mol	NIST Webbook
ie	7.70	eV	NIST Webbook
ie	7.37 ± 0.05	eV	NIST Webbook
log10ws	-6.96		Estimated Solubility Method
log10ws	-6.96		Aqueous Solubility Prediction Method
logp	4.301		Crippen Method
mcvol	159.530	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	321.16		NIST Webbook
rinpol	1920.70		NIST Webbook
rinpol	1928.00		NIST Webbook
rinpol	1872.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1883.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1878.00		NIST Webbook
rinpol	1905.00		NIST Webbook
rinpol	1955.00		NIST Webbook

rinpol	316.50		NIST Webbook
rinpol	317.80		NIST Webbook
rinpol	321.57		NIST Webbook
rinpol	320.90		NIST Webbook
rinpol	321.14		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	320.88		NIST Webbook
rinpol	321.38		NIST Webbook
rinpol	321.08		NIST Webbook
rinpol	320.96		NIST Webbook
rinpol	321.14		NIST Webbook
rinpol	321.47		NIST Webbook
rinpol	321.41		NIST Webbook
rinpol	321.57		NIST Webbook
rinpol	321.12		NIST Webbook
rinpol	321.12		NIST Webbook
rinpol	321.14		NIST Webbook
rinpol	321.57		NIST Webbook
rinpol	341.82		NIST Webbook
rinpol	320.39		NIST Webbook
rinpol	320.90		NIST Webbook
rinpol	321.60		NIST Webbook
rinpol	320.90		NIST Webbook
rinpol	321.57		NIST Webbook
rinpol	322.10		NIST Webbook
rinpol	319.42		NIST Webbook
rinpol	319.76		NIST Webbook
rinpol	321.57		NIST Webbook
rinpol	1883.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1905.00		NIST Webbook
rinpol	1920.70		NIST Webbook
rinpol	1930.00		NIST Webbook
tb	617.20	K	Joback Method
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	0.0005079	Pa×s	576.95	Joback Method
dvisc	0.0005828	Pa×s	536.69	Joback Method
dvisc	0.0006839	Pa×s	496.44	Joback Method
dvisc	0.0008255	Pa×s	456.18	Joback Method
dvisc	0.0010334	Pa×s	415.93	Joback Method
dvisc	0.0004506	Pa×s	617.20	Joback Method
dvisc	0.0013574	Pa×s	375.67	Joback Method
hvapt	76.10	kJ/mol	398.00	NIST Webbook
pvap	2.75e-03	kPa	350.00	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	0.02	kPa	380.00	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	1.23e-03	kPa	340.00	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	0.20	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.33	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.51	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.78	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.15	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.67	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.37	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.30	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.52	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.08	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	5.18e-04	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.04e-04	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	7.48e-05	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.53e-05	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.05e-05	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	5.81e-03	kPa	360.00	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.29200e+01
Coeff. B	-4.27355e+03
Coeff. C	-1.16618e+02
Temperature range (K), min.	454.92

Temperature range (K), max.	678.30

Sources

Solubilities of Triptycene, 9-Phenylanthracene, 9,10-Dimethylanthracene, and 2-Methylanthracene in Pressurized Hot Water at Temperatures from 313 K to the Melting Point:	https://www.doi.org/10.1021/je700447m
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
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=C613127&Units=SI
Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:	https://www.doi.org/10.1021/je800300x
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

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