

Anthracene, 9-methyl-

Other names:	9-Methylantracene
Inchi:	InChI=1S/C15H12/c1-11-14-8-4-2-6-12(14)10-13-7-3-5-9-15(11)13/h2-10H,1H3
InchiKey:	CPGPAVAKSZHMBP-UHFFFAOYSA-N
Formula:	C15H12
SMILES:	<chem>Cc1c2ccccc2cc2ccccc12</chem>
Mol. weight [g/mol]:	192.26
CAS:	779-02-2

Physical Properties

Property code	Value	Unit	Source
affp	896.50	kJ/mol	NIST Webbook
affp	893.70	kJ/mol	NIST Webbook
basg	865.70	kJ/mol	NIST Webbook
basg	865.80	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
hsub	101.80 ± 1.00	kJ/mol	NIST Webbook
hvap	88.10 ± 1.00	kJ/mol	NIST Webbook
ie	7.25	eV	NIST Webbook
ie	7.24 ± 0.03	eV	NIST Webbook
ie	7.27	eV	NIST Webbook
ie	7.24 ± 0.03	eV	NIST Webbook
ie	7.46 ± 0.03	eV	NIST Webbook
ie	7.31 ± 0.05	eV	NIST Webbook
log10ws	-5.89		Aqueous Solubility Prediction Method
log10ws	-5.89		Estimated Solubility Method
logp	4.301		Crippen Method
mcvol	159.530	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	329.09		NIST Webbook
rinpol	1926.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	312.30		NIST Webbook
rinpol	309.19		NIST Webbook
rinpol	1941.20		NIST Webbook

rinpol	329.36		NIST Webbook
rinpol	329.52		NIST Webbook
rinpol	329.13		NIST Webbook
rinpol	309.70		NIST Webbook
rinpol	330.10		NIST Webbook
rinpol	324.16		NIST Webbook
rinpol	327.74		NIST Webbook
rinpol	329.13		NIST Webbook
rinpol	1999.00		NIST Webbook
rinpol	1999.00		NIST Webbook
rinpol	1999.00		NIST Webbook
tb	617.20	K	Joback Method
tc	866.35	K	Joback Method
tf	352.53	K	Aqueous Solubility Prediction Method
tf	354.00 ± 4.00	K	NIST Webbook
tf	354.00 ± 2.00	K	NIST Webbook
tf	354.80	K	Thermochemistry of some alkylsubstituted anthracenes
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.90	J/molxK	866.35	Joback Method
cpg	396.50	J/molxK	658.73	Joback Method
cpg	410.54	J/molxK	700.25	Joback Method
cpg	423.46	J/molxK	741.78	Joback Method
cpg	435.41	J/molxK	783.30	Joback Method
cpg	446.52	J/molxK	824.83	Joback Method
cpg	381.22	J/molxK	617.20	Joback Method
dvisc	0.0005079	Paxs	576.95	Joback Method
dvisc	0.0005828	Paxs	536.69	Joback Method
dvisc	0.0006839	Paxs	496.44	Joback Method
dvisc	0.0008255	Paxs	456.18	Joback Method
dvisc	0.0010334	Paxs	415.93	Joback Method
dvisc	0.0004506	Paxs	617.20	Joback Method
dvisc	0.0013574	Paxs	375.67	Joback Method
hsubt	99.80 ± 1.00	kJ/mol	337.00	NIST Webbook
hvapt	56.50	kJ/mol	469.00	NIST Webbook
hvapt	98.90	kJ/mol	378.00	NIST Webbook

hvapt	58.50	kJ/mol	505.00	NIST Webbook	
hvapt	58.10	kJ/mol	469.00	NIST Webbook	
pvap	4.19e-05	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons	
pvap	8.20e-03	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons	
pvap	1.34e-05	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons	
pvap	0.03	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons	
pvap	0.05	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons	
pvap	0.09	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons	

pvap	0.16	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.26	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.41	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.62	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.93	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.35	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.93	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	2.69	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.69	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.97	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.08e-05	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.97e-03	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.82e-03	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.86e-04	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	3.18e-04	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.20e-04	kPa	320.00	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	469.70	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.29219e+01
Coeff. B	-4.27451e+03
Coeff. C	-1.16618e+02
Temperature range (K), min.	454.94
Temperature range (K), max.	678.28

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polycyclic Aromatic 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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermochemistry of some alkylsubstituted anthracenes:	https://www.doi.org/10.1016/j.jct.2005.06.001
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C779022&Units=SI

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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