9H-Fluorene, 1-methyl-

Other names:	1-Methylfluorene
	1-methyl-9H-fluorene
	Fluorene, 1-methyl-
Inchi:	InChI=1S/C14H12/c1-10-5-4-8-13-12-7-3-2-6-11(12)9-14(10)13/h2-8H,9H2,1H3
InchiKey:	GKEUODMJRFDLJY-UHFFFAOYSA-N
Formula:	C14H12
SMILES:	Cc1cccc2c1Cc1ccccc1-2
Mol. weight [g/mol]:	180.25
CAS:	1730-37-6

Physical Properties

Property code	Value	Unit	Source
gf	355.59	kJ/mol	Joback Method
hf	211.82	kJ/mol	Joback Method
hfus	20.20	kJ/mol	Joback Method
hsub	91.20 ± 0.40	kJ/mol	NIST Webbook
hvap	78.70 ± 0.70	kJ/mol	NIST Webbook
hvap	77.20 ± 3.60	kJ/mol	NIST Webbook
log10ws	-5.22		Aqueous Solubility Prediction Method
log10ws	-5.22		Estimated Solubility Method
logp	3.566		Crippen Method
mcvol	149.740	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	289.31		NIST Webbook
rinpol	289.27		NIST Webbook
rinpol	290.45		NIST Webbook
rinpol	289.07		NIST Webbook
rinpol	287.70		NIST Webbook
rinpol	290.39		NIST Webbook
rinpol	289.50		NIST Webbook
rinpol	288.70		NIST Webbook
rinpol	288.80		NIST Webbook
rinpol	289.14		NIST Webbook
rinpol	289.49		NIST Webbook
rinpol	289.20		NIST Webbook
rinpol	289.03		NIST Webbook

rinpol	289.24		NIST Webbook
rinpol	289.14		NIST Webbook
rinpol	289.24		NIST Webbook
rinpol	289.30		NIST Webbook
rinpol	289.03		NIST Webbook
rinpol	288.70		NIST Webbook
rinpol	289.00		NIST Webbook
rinpol	288.70		NIST Webbook
rinpol	289.03		NIST Webbook
rinpol	289.20		NIST Webbook
rinpol	289.30		NIST Webbook
rinpol	289.03		NIST Webbook
rinpol	290.55		NIST Webbook
rinpol	1698.20		NIST Webbook
rinpol	290.70		NIST Webbook
rinpol	288.57		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1718.80		NIST Webbook
rinpol	1698.20		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	290.20		NIST Webbook
rinpol	1680.00		NIST Webbook
ripol	2475.00		NIST Webbook
ripol	2406.00		NIST Webbook
ripol	2406.00		NIST Webbook
tb	590.89	K	Joback Method
tc	834.31	K	Joback Method
tf	367.16	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.92	J/mol×K	590.89	Joback Method
cpg	367.90	J/mol×K	631.46	Joback Method
cpg	381.68	J/mol×K	672.03	Joback Method
cpg	394.39	J/mol×K	712.60	Joback Method
cpg	406.16	J/mol×K	753.17	Joback Method

cpg	417.12	J/mol×K	793.74	Joback Method
cpg	427.40	J/mol×K	834.31	Joback Method
dvisc	0.0013988	Pa×s	367.16	Joback Method
dvisc	0.0011308	Pa×s	404.45	Joback Method
dvisc	0.0009476	Pa×s	441.74	Joback Method
dvisc	0.0008162	Pa×s	479.02	Joback Method
dvisc	0.0007184	Pa×s	516.31	Joback Method
dvisc	0.0006433	Pa×s	553.60	Joback Method
dvisc	0.0005841	Pa×s	590.89	Joback Method
hvapt	71.10	kJ/mol	398.00	NIST Webbook
pvap	2.72e-03	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.69e-04	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.60e-04	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.16e-03	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.40e-04	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	6.01e-03	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.01	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.02	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.05	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.08	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.15	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.25	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.40	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.63	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.97	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.44	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.10	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.99	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.17	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	5.72	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.69	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	10.18	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	13.27	kPa	510.00	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	1.26883e+01
Coeff. B	-3.92926e+03
Coeff. C	-9.93270e+01
Temperature range (K), min.	416.19
Temperature range (K), max.	631.98

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1730376&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
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

Legend

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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume