Pyrene, 1-methyl-

Other names:	1-Methylpyrene
	3-Methylpyrene
	Pyrene, 3-methyl
Inchi:	InChI=1S/C17H12/c1-11-5-6-14-8-7-12-3-2-4-13-9-10-15(11)17(14)16(12)13/h2-10H,1H3
InchiKey:	KBSPJIWZDWBDGM-UHFFFAOYSA-N
Formula:	C17H12
SMILES:	Cc1ccc2ccc3cccc4ccc1c2c34
Mol. weight [g/mol]:	216.28
CAS:	2381-21-7

Physical Properties

Property code	Value	Unit	Source
gf	489.97	kJ/mol	Joback Method
hf	335.66	kJ/mol	Joback Method
hfus	26.70	kJ/mol	Joback Method
hvap	92.30 ± 1.30	kJ/mol	NIST Webbook
log10ws	-6.78		Crippen Method
logp	4.892		Crippen Method
mcvol	172.550	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	370.29		NIST Webbook
rinpol	374.20		NIST Webbook
rinpol	374.43		NIST Webbook
rinpol	373.23		NIST Webbook
rinpol	373.27		NIST Webbook
rinpol	373.44		NIST Webbook
rinpol	373.55		NIST Webbook
rinpol	374.30		NIST Webbook
rinpol	373.72		NIST Webbook
rinpol	373.45		NIST Webbook
rinpol	373.55		NIST Webbook
rinpol	373.40		NIST Webbook
rinpol	373.55		NIST Webbook
rinpol	373.45		NIST Webbook
rinpol	373.55		NIST Webbook
rinpol	373.72		NIST Webbook
rinpol	370.00		NIST Webbook

rinpol	415.27		NIST Webbook
rinpol	373.60		NIST Webbook
rinpol	374.20		NIST Webbook
rinpol	371.86		NIST Webbook
rinpol	372.57		NIST Webbook
rinpol	373.55		NIST Webbook
rinpol	368.09		NIST Webbook
rinpol	370.88		NIST Webbook
rinpol	371.43		NIST Webbook
rinpol	371.73		NIST Webbook
rinpol	373.00		NIST Webbook
rinpol	373.55		NIST Webbook
rinpol	368.09		NIST Webbook
rinpol	370.65		NIST Webbook
rinpol	372.88		NIST Webbook
rinpol	370.29		NIST Webbook
rinpol	373.40		NIST Webbook
rinpol	370.00		NIST Webbook
rinpol	372.97		NIST Webbook
rinpol	371.73		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	373.55		NIST Webbook
rinpol	373.44		NIST Webbook
rinpol	2212.00		NIST Webbook
rinpol	2215.00		NIST Webbook
rinpol	2212.00		NIST Webbook
rinpol	372.88		NIST Webbook
rinpol	372.97		NIST Webbook
rinpol	373.05		NIST Webbook
tb	679.22	K	Joback Method
tc	930.34	K	Joback Method
tf	347.65 ± 2.00	K	NIST Webbook
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.75	J/mol×K	679.22	Joback Method
cpg	449.48	J/mol×K	721.07	Joback Method
cpg	462.19	J/mol×K	762.93	Joback Method
cpg	474.06	J/mol×K	804.78	Joback Method

cpg	485.29	J/mol×K	846.63	Joback Method
cpg	496.08	J/mol×K	888.49	Joback Method
cpg	506.62	J/mol×K	930.34	Joback Method
dvisc	0.0019946	Pa×s	449.71	Joback Method
dvisc	0.0018069	Pa×s	487.96	Joback Method
dvisc	0.0016605	Pa×s	526.21	Joback Method
dvisc	0.0015435	Pa×s	564.47	Joback Method
dvisc	0.0014482	Pa×s	602.72	Joback Method
dvisc	0.0013691	Pa×s	640.97	Joback Method
dvisc	0.0013026	Pa×s	679.22	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37781e+01
Coeff. B	-5.05699e+03
Coeff. C	-1.31066e+02
Temperature range (K), min.	505.92
Temperature range (K), max.	728.35

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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=C2381217&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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