1,3-Cyclopentadiene, 1-methyl-

Other names:	1-Methyl-1,3-cyclopentadiene
	1-Methylcyclopentadiene
	Methylcyclopentadiene
	l,3-Cyclopentadiene,1-methyl-
Inchi:	InChI=1S/C6H8/c1-6-4-2-3-5-6/h2-4H,5H2,1H3
InchiKey:	NFWSQSCIDYBUOU-UHFFFAOYSA-N
Formula:	C6H8
SMILES:	CC1=CC=CC1
Mol. weight [g/mol]:	80.13
CAS:	96-39-9

Physical Properties

Property code	Value	Unit	Source
gf	94.19	kJ/mol	Joback Method
hf	17.74	kJ/mol	Joback Method
hfus	6.22	kJ/mol	Joback Method
hvap	30.76	kJ/mol	Joback Method
ie	8.43 ± 0.05	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.40 ± 0.02	eV	NIST Webbook
ie	8.40 ± 0.02	eV	NIST Webbook
log10ws	-1.94		Crippen Method
logp	1.893		Crippen Method
mcvol	75.940	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
rinpol	626.30		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	644.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	627.50		NIST Webbook
rinpol	653.80		NIST Webbook
rinpol	652.80		NIST Webbook
rinpol	644.00		NIST Webbook

rinpol	641.00		NIST Webbook
rinpol	644.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	623.00		NIST Webbook
ripol	844.50		NIST Webbook
tb	359.93	K	Joback Method
tc	561.67	K	Joback Method
tf	186.56	K	Joback Method
tt	130.20 ± 0.10	K	NIST Webbook
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.91	J/mol×K	359.93	Joback Method
cpg	127.40	J/mol×K	393.55	Joback Method
cpg	137.29	J/mol×K	427.18	Joback Method
cpg	146.63	J/mol×K	460.80	Joback Method
cpg	155.42	J/mol×K	494.42	Joback Method
cpg	163.69	J/mol×K	528.04	Joback Method
cpg	171.48	J/mol×K	561.67	Joback Method
dvisc	0.0018579	Pa×s	186.56	Joback Method
dvisc	0.0010520	Pa×s	215.45	Joback Method
dvisc	0.0006814	Pa×s	244.35	Joback Method
dvisc	0.0004838	Pa×s	273.25	Joback Method
dvisc	0.0003668	Pa×s	302.14	Joback Method
dvisc	0.0002919	Pa×s	331.03	Joback Method
dvisc	0.0002409	Pa×s	359.93	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.35325e+01
Coeff. B	-5.50987e+03

Coeff. C	-5.71400e+00
Coeff. D	3.37471e-06
Temperature range (K), min.	150.00
Temperature range (K), max.	541.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol610.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96399&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=610
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
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume