1,3-Cyclopentadiene

Other names:	CYCLOPENTADIENE
	PENTOLE
	PYROPENTYLENE
	R-PENTINE
Inchi:	InChI=1S/C5H6/c1-2-4-5-3-1/h1-4H,5H2
InchiKey:	ZSWFCLXCOIISFI-UHFFFAOYSA-N
Formula:	C5H6
SMILES:	C1=CCC=C1
Mol. weight [g/mol]:	66.10
CAS:	542-92-7

Physical Properties

Property code	Value	Unit	Source
affp	828.00	kJ/mol	NIST Webbook
affp	821.60	kJ/mol	NIST Webbook
basg	798.40	kJ/mol	NIST Webbook
basg	798.30	kJ/mol	NIST Webbook
chg	-2960.00 ± 30.00	kJ/mol	NIST Webbook
gf	95.40	kJ/mol	Joback Method
hf	139.00	kJ/mol	NIST Webbook
hf	133.40	kJ/mol	NIST Webbook
hfus	4.01	kJ/mol	Joback Method
hvap	29.70	kJ/mol	NIST Webbook
hvap	29.00	kJ/mol	NIST Webbook
hvap	28.40 ± 0.30	kJ/mol	NIST Webbook
hvap	28.40 ± 0.30	kJ/mol	NIST Webbook
ie	8.57 ± 0.01	eV	NIST Webbook
ie	8.56 ± 0.01	eV	NIST Webbook
ie	8.58 ± 0.02	eV	NIST Webbook
ie	8.56	eV	NIST Webbook
ie	8.57 ± 0.01	eV	NIST Webbook
ie	8.44	eV	NIST Webbook
ie	8.53	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	8.57 ± 0.01	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.55	eV	NIST Webbook

ie	8.61	eV	NIST Webbook
log10ws	-1.52		Crippen Method
logp	1.502		Crippen Method
mcvol	61.850	ml/mol	McGowan Method
pc	5008.59	kPa	Joback Method
rinpol	527.00		NIST Webbook
rinpol	510.50		NIST Webbook
rinpol	552.50		NIST Webbook
rinpol	549.50		NIST Webbook
rinpol	534.70		NIST Webbook
rinpol	521.70		NIST Webbook
rinpol	543.00		NIST Webbook
rinpol	541.00		NIST Webbook
rinpol	545.00		NIST Webbook
rinpol	542.00		NIST Webbook
rinpol	523.00		NIST Webbook
rinpol	546.00		NIST Webbook
rinpol	540.00		NIST Webbook
rinpol	521.80		NIST Webbook
rinpol	542.00		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	520.60		NIST Webbook
rinpol	516.61		NIST Webbook
rinpol	519.00		NIST Webbook
rinpol	522.00		NIST Webbook
rinpol	528.00		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	538.10		NIST Webbook
rinpol	533.00		NIST Webbook
rinpol	522.00		NIST Webbook
rinpol	528.00		NIST Webbook
rinpol	525.00		NIST Webbook
rinpol	523.00		NIST Webbook
rinpol	538.00		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	535.00		NIST Webbook
rinpol	540.00		NIST Webbook
rinpol	97.20		NIST Webbook
rinpol	545.00		NIST Webbook
rinpol	538.10		NIST Webbook
rinpol	521.60		NIST Webbook

rinpol	523.00		NIST Webbook
ripol	745.70		NIST Webbook
ripol	735.00		NIST Webbook
sg	274.47	J/mol×K	NIST Webbook
sl	182.70	J/mol×K	NIST Webbook
tb	313.00 ± 2.00	K	NIST Webbook
tb	315.70 ± 3.00	K	NIST Webbook
tb	314.00 ± 3.00	K	NIST Webbook
tb	314.90 ± 2.00	K	NIST Webbook
tb	314.20 ± 5.00	K	NIST Webbook
tb	313.15 ± 2.00	K	NIST Webbook
tb	313.90 ± 2.00	K	NIST Webbook
tb	313.20	K	NIST Webbook
tc	532.62	K	Joback Method
tf	183.15 ± 10.00	K	NIST Webbook
tf	188.00 ± 3.00	K	NIST Webbook
tt	176.60 ± 0.05	K	NIST Webbook
vc	0.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.85	J/mol×K	532.62	Joback Method
cpg	81.65	J/mol×K	332.07	Joback Method
cpg	108.71	J/mol×K	432.34	Joback Method
cpg	116.60	J/mol×K	465.77	Joback Method
cpg	123.97	J/mol×K	499.19	Joback Method
cpg	100.27	J/mol×K	398.92	Joback Method
cpg	91.26	J/mol×K	365.49	Joback Method
cpl	115.30	J/mol×K	298.15	NIST Webbook
dvisc	0.0002333	Pa×s	332.07	Joback Method
dvisc	0.0003700	Pa×s	275.64	Joback Method
dvisc	0.0005043	Pa×s	247.42	Joback Method
dvisc	0.0007443	Pa×s	219.20	Joback Method
dvisc	0.0012326	Pa×s	190.99	Joback Method
dvisc	0.0002876	Pa×s	303.85	Joback Method
dvisc	0.0024310	Pa×s	162.77	Joback Method
hfust	8.01	kJ/mol	176.60	NIST Webbook
hfust	8.01	kJ/mol	176.60	NIST Webbook
hvapt	28.10	kJ/mol	302.50	NIST Webbook
hvapt	28.20	kJ/mol	292.50	NIST Webbook

sfust	45.40	J/mol×K	176.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47937e+01
Coeff. B	-3.06948e+03
Coeff. C	-1.23430e+01
Temperature range (K), min.	223.94
Temperature range (K), max.	336.05

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.26203e+01
Coeff. B	-4.93279e+03
Coeff. C	-7.52765e+00
Coeff. D	9.77663e-06
Temperature range (K), min.	188.15
Temperature range (K), max.	507.00

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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol608.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C542927&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=608

Legend

affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion 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
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume