Cyclopentene, 3-methyl-

Other names:	3-Methyl-1-cyclopentene
	3-Methylcyclopentene
	3-Methylcyclopentene-1
Inchi:	InChI=1S/C6H10/c1-6-4-2-3-5-6/h2,4,6H,3,5H2,1H3
InchiKey:	CXOZQHPXKPDQGT-UHFFFAOYSA-N
Formula:	C6H10
SMILES:	CC1C=CCC1
Mol. weight [g/mol]:	82.14
CAS:	1120-62-3

Physical Properties

Property code	Value	Unit	Source
af	0.2210		KDB
chl	-3766.50 ± 0.54	kJ/mol	NIST Webbook
gf	66.15	kJ/mol	Joback Method
hcg	3766.52	kJ/mol	KDB
hcn	3546.442	kJ/mol	KDB
hf	7.36 ± 0.71	kJ/mol	NIST Webbook
hf	9.67	kJ/mol	NIST Webbook
hf	8.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-24.90 ± 1.80	kJ/mol	NIST Webbook
hfus	6.45	kJ/mol	Joback Method
hvap	32.90	kJ/mol	NIST Webbook
hvap	31.00 ± 0.20	kJ/mol	NIST Webbook
hvap	31.00 ± 0.30	kJ/mol	NIST Webbook
hvap	32.00 ± 2.00	kJ/mol	NIST Webbook
ie	8.95 ± 0.01	eV	NIST Webbook
ie	8.95	eV	NIST Webbook
ie	8.99 ± 0.04	eV	NIST Webbook
ie	8.98 ± 0.05	eV	NIST Webbook
log10ws	-1.84		Crippen Method
logp	1.973		Crippen Method
mcvol	80.240	ml/mol	McGowan Method
pc	4020.00	kPa	KDB
rinpol	605.80		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	608.00		NIST Webbook

rinpol	601.00	NIST Webbook
rinpol	602.00	NIST Webbook
rinpol	627.00	NIST Webbook
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rinpol	633.00	NIST Webbook
rinpol	601.50	NIST Webbook
rinpol	619.00	NIST Webbook
rinpol	607.70	NIST Webbook
rinpol	602.00	NIST Webbook
rinpol	606.00	NIST Webbook
rinpol	608.00	NIST Webbook
rinpol	615.00	NIST Webbook
rinpol	609.00	NIST Webbook
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rinpol	611.40	NIST Webbook
rinpol	637.44	NIST Webbook
rinpol	620.00	NIST Webbook
rinpol	610.00	NIST Webbook
rinpol	588.00	NIST Webbook
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rinpol	619.00		NIST Webbook
rinpol	598.00		NIST Webbook
rinpol	619.00		NIST Webbook
rinpol	598.00		NIST Webbook
rinpol	610.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	607.00		NIST Webbook
rinpol	615.00		NIST Webbook
ripol	736.00		NIST Webbook
ripol	725.60		NIST Webbook
ripol	736.00		NIST Webbook
ripol	728.70		NIST Webbook
ripol	725.60		NIST Webbook
ripol	735.80		NIST Webbook
ripol	728.70		NIST Webbook
ripol	725.60		NIST Webbook
ripol	735.80		NIST Webbook
ripol	736.00		NIST Webbook
ripol	729.00		NIST Webbook
ripol	726.00		NIST Webbook
tb	343.20	K	KDB
tc	535.70	K	KDB
tf	130.00	K	KDB
vc	0.298	m3/kmol	KDB
zc	0.2694090		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.84	J/mol×K	515.30	Joback Method
cpg	125.84	J/mol×K	351.12	Joback Method
cpg	138.48	J/mol×K	383.96	Joback Method
cpg	150.48	J/mol×K	416.79	Joback Method

cpg	161.86	J/mol×K	449.63	Joback Method
cpg	172.64	J/mol×K	482.46	Joback Method
cpg	192.49	J/mol×K	548.13	Joback Method
cpl	152.30	J/mol×K	298.15	NIST Webbook
dvisc	0.0002498	Pa×s	351.12	Joback Method
dvisc	0.0020778	Pa×s	169.04	Joback Method
dvisc	0.0011158	Pa×s	199.39	Joback Method
dvisc	0.0007062	Pa×s	229.73	Joback Method
dvisc	0.0004973	Pa×s	260.08	Joback Method
dvisc	0.0003768	Pa×s	290.43	Joback Method
dvisc	0.0003009	Pa×s	320.77	Joback Method
hvapt	32.10	kJ/mol	327.50	NIST Webbook
rfi	1.41840		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47876e+01
Coeff. B	-3.34343e+03
Coeff. C	-1.02240e+01
Temperature range (K), min.	240.80
Temperature range (K), max.	363.05

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.22594e+01
Coeff. B	-5.95667e+03
Coeff. C	-8.74178e+00
Coeff. D	7.71533e-06
Temperature range (K), min.	263.15
Temperature range (K), max.	392.15

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=612
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/research/kdb/hcprop/showprop.php?cmpid=612
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1120623&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
rfi:	Refractive Index
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
zc:	Critical Compressibility

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