

Cyclopentene, 4-methyl-

Other names:	1-METHYL-3-CYCLOPENTENE 4-Methylcyclopentene
Inchi:	InChI=1S/C6H10/c1-6-4-2-3-5-6/h2-3,6H,4-5H2,1H3
InchiKey:	FWMRUAODTCVEQK-UHFFFAOYSA-N
Formula:	C6H10
SMILES:	CC1CC=CC1
Mol. weight [g/mol]:	82.14
CAS:	1759-81-5

Physical Properties

Property code	Value	Unit	Source
af	0.2210		KDB
chl	-3772.60 ± 1.00	kJ/mol	NIST Webbook
gf	66.15	kJ/mol	Joback Method
hcg	3772.63	kJ/mol	KDB
hcn	3552.551	kJ/mol	KDB
hf	15.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-17.70 ± 1.00	kJ/mol	NIST Webbook
hfus	6.45	kJ/mol	Joback Method
hvap	32.70	kJ/mol	NIST Webbook
hvap	32.00 ± 2.00	kJ/mol	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	610.00		NIST Webbook
rinpol	610.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	610.00		NIST Webbook
rinpol	610.00		NIST Webbook
tb	338.30 ± 0.50	K	NIST Webbook
tb	345.20 ± 4.00	K	NIST Webbook
tb	348.70 ± 1.50	K	NIST Webbook
tb	348.00 ± 6.00	K	NIST Webbook
tb	348.30	K	KDB
tc	543.80	K	KDB
tf	146.06 ± 0.30	K	NIST Webbook

tf	112.00	K	KDB
vc	0.298	m3/kmol	KDB
zc	0.2653960		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	182.84	J/mol×K	515.30	Joback Method
cpg	192.49	J/mol×K	548.13	Joback Method
dvisc	0.0011158	Pa×s	199.39	Joback Method
dvisc	0.0020778	Pa×s	169.04	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
dvisc	0.0002498	Pa×s	351.12	Joback Method
hvapt	33.20	kJ/mol	337.00	NIST Webbook
rfi	1.41840		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43862e+01
Coeff. B	-2.89521e+03
Coeff. C	-4.18990e+01
Temperature range (K), min.	247.25
Temperature range (K), max.	360.94

Information	Value
Property code	pvap

Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	6.76639e+01
Coeff. B	-5.96721e+03
Coeff. C	-7.97289e+00
Coeff. D	6.19549e-06
Temperature range (K), min.	271.15
Temperature range (K), max.	543.75

Sources

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/mol613.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1759815&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=613
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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