Cyclopentane, 1,1-dimethyl-

Other names: 1,1-Dimethylcyclopentane
GEM-DIMETHYLCYCLOPENTANE
Inchi: InChI=1S/C7H14/c1-7(2)5-3-4-6-7/h3-6H2,1-2H3
InchiKey: QWHNJUXXYKPLQM-UHFFFAOYSA-N
Formula: C7H14
SMILES: CC1(C)CCCC1
Mol. weight [g/mol]: 98.19
CAS: 1638-26-2

Physical Properties

Property code	Value	Unit	Source
af	0.2730		KDB
ap	318.150	K	KDB
chl	-4583.30 ± 1.00	kJ/mol	NIST Webbook
gf	39.06	kJ/mol	KDB
hcg	4583.32	kJ/mol	KDB
hcn	4275.253	kJ/mol	KDB
hf	-138.40	kJ/mol	KDB
hf	-138.30 ± 1.20	kJ/mol	NIST Webbook
hfl	-172.10 ± 1.10	kJ/mol	NIST Webbook
hfus	1.52	kJ/mol	Joback Method
hvap	33.80	kJ/mol	NIST Webbook
hvap	33.80	kJ/mol	NIST Webbook
ie	9.46 ± 0.05	eV	NIST Webbook
log10ws	-2.41		Crippen Method
logp	2.587		Crippen Method
mcvol	98.630	ml/mol	McGowan Method
pc	3440.00	kPa	KDB
rinpol	671.10		NIST Webbook
rinpol	665.59		NIST Webbook
rinpol	669.70		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	675.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	673.00		NIST Webbook
rinpol	669.00		NIST Webbook
rinpol	665.00		NIST Webbook

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rinpol	673.00	NIST Webbook
rinpol	670.00	NIST Webbook
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rinpol	666.00	NIST Webbook
rinpol	665.63	NIST Webbook
rinpol	665.48	NIST Webbook
rinpol	665.59	NIST Webbook
rinpol	676.80	NIST Webbook
rinpol	671.00	NIST Webbook
rinpol	675.00	NIST Webbook
rinpol	675.40	NIST Webbook
rinpol	674.00	NIST Webbook
rinpol	684.00	NIST Webbook
rinpol	672.00	NIST Webbook
rinpol	665.52	NIST Webbook
rinpol	668.50	NIST Webbook
rinpol	663.04	NIST Webbook
rinpol	662.30	NIST Webbook
rinpol	677.00	NIST Webbook
rinpol	665.00	NIST Webbook
rinpol	675.50	NIST Webbook
rinpol	669.00	NIST Webbook
rinpol	675.90	NIST Webbook
rinpol	676.00	NIST Webbook
rinpol	676.80	NIST Webbook
rinpol	676.10	NIST Webbook
rinpol	675.80	NIST Webbook
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rinpol	676.10		NIST Webbook
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rinpol	674.00		NIST Webbook
rinpol	672.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	669.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	677.00		NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	677.00		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	669.70		NIST Webbook
sg	359.28	J/mol×K	NIST Webbook
sl	265.01	J/mol×K	NIST Webbook
tb	361.35 ± 0.30	K	NIST Webbook
tb	361.00 ± 0.20	K	NIST Webbook
tb	361.05 ± 0.30	K	NIST Webbook
tb	361.20 ± 0.30	K	NIST Webbook

tb	360.65 ± 0.50	K	NIST Webbook
tb	360.70 ± 0.30	K	NIST Webbook
tb	360.00 ± 1.00	K	NIST Webbook
tb	360.70	K	NIST Webbook
tb	361.00	K	KDB
tb	360.99 ± 0.02	K	NIST Webbook
tb	361.30 ± 0.60	K	NIST Webbook
tb	360.65 ± 0.20	K	NIST Webbook
tc	547.00	K	KDB
tf	203.35 ± 0.05	K	NIST Webbook
tf	203.42 ± 0.06	K	NIST Webbook
tf	203.24 ± 0.20	K	NIST Webbook
tf	203.24 ± 0.30	K	NIST Webbook
tf	203.40	K	KDB
tf	203.34 ± 0.08	K	NIST Webbook
tf	203.24 ± 0.30	K	NIST Webbook
tf	203.42 ± 0.10	K	NIST Webbook
tf	197.28 ± 4.00	K	NIST Webbook
tf	203.16 ± 1.00	K	NIST Webbook
tf	196.75 ± 0.40	K	NIST Webbook
tf	196.75 ± 5.00	K	NIST Webbook
tf	196.00 ± 5.00	K	NIST Webbook
tf	203.34 ± 0.07	K	NIST Webbook
tf	203.27 ± 0.20	K	NIST Webbook
tt	203.68 ± 0.05	K	NIST Webbook
tt	203.67 ± 0.02	K	NIST Webbook
tt	203.67 ± 0.03	K	NIST Webbook
tt	203.67 ± 0.02	K	NIST Webbook
vc	0.360	m3/kmol	KDB
zc	0.2722930		KDB
zra	0.28		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.34	J/mol×K	375.08	Joback Method
cpg	205.94	J/mol×K	442.81	Joback Method
cpg	190.73	J/mol×K	408.95	Joback Method
cpg	256.90	J/mol×K	578.27	Joback Method
cpg	245.45	J/mol×K	544.41	Joback Method
cpg	233.21	J/mol×K	510.54	Joback Method

cpg	220.07	J/mol×K	476.68	Joback Method
cpl	187.36	J/mol×K	299.81	NIST Webbook
hfust	6.49	kJ/mol	146.80	NIST Webbook
hfust	1.09	kJ/mol	203.70	NIST Webbook
hfust	1.09	kJ/mol	203.70	NIST Webbook
hvapt	33.80	kJ/mol	325.50	NIST Webbook
hvapt	34.00	kJ/mol	323.50	NIST Webbook
hvapt	30.29	kJ/mol	361.00	KDB
rfi	1.41091		298.15	KDB
rhol	759.00	kg/m3	289.00	KDB
sfust	44.18	J/mol×K	146.80	NIST Webbook
sfust	5.34	J/mol×K	203.70	NIST Webbook
srf	0.02	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42167e+01
Coeff. B	-3.06828e+03
Coeff. C	-4.12340e+01
Temperature range (K), min.	261.51
Temperature range (K), max.	385.78

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.87017e+01
Coeff. B	-6.92875e+03
Coeff. C	-1.12381e+01
Coeff. D	9.90988e-06
Temperature range (K), min.	203.36
Temperature range (K), max.	547.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1638262&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=472
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/mol472.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
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
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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-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
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter