

Cyclopentane, 1,2-dimethyl-, trans-

Other names:	(E)-1,2-Dimethylcyclopentane 1,2-Dimethylcyclopentane, trans 1,TRANS-2-DIMETHYLCYCLOPENTANE Cyclopentane, 1,2-dimethyl- TRANS-1,2-DIMETHYLCYCLOPENTANE t-1,2-Dimethylcyclopentane
Inchi:	InChI=1S/C7H14/c1-6-4-3-5-7(6)2/h6-7H,3-5H2,1-2H3/t6-,7-/m0/s1
InchiKey:	RIRARCHMRDHZAR-BQBZGAKWSA-N
Formula:	C7H14
SMILES:	CC1CCCC1C
Mol. weight [g/mol]:	98.19
CAS:	822-50-4

Physical Properties

Property code	Value	Unit	Source
af	0.2690		KDB
ap	319.850	K	KDB
chl	-4584.20 ± 1.10	kJ/mol	NIST Webbook
gf	38.39	kJ/mol	KDB
hcg	4584.16	kJ/mol	KDB
hcn	4276.090	kJ/mol	KDB
hf	-136.70 ± 1.30	kJ/mol	NIST Webbook
hf	-136.80	kJ/mol	KDB
hfl	-171.30 ± 1.20	kJ/mol	NIST Webbook
hfus	8.89	kJ/mol	Joback Method
hvap	34.60	kJ/mol	NIST Webbook
hvap	34.60	kJ/mol	NIST Webbook
ie	9.48 ± 0.05	eV	NIST Webbook
ie	9.95 ± 0.05	eV	NIST Webbook
log10ws	-2.16		Crippen Method
logp	2.442		Crippen Method
mcvol	98.630	ml/mol	McGowan Method
pc	3440.00	kPa	KDB
rinpol	693.00		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	686.60		NIST Webbook

rinpol	684.12	NIST Webbook
rinpol	692.00	NIST Webbook
rinpol	691.60	NIST Webbook
rinpol	685.60	NIST Webbook
rinpol	689.10	NIST Webbook
rinpol	694.10	NIST Webbook
rinpol	685.00	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	691.00	NIST Webbook
rinpol	691.00	NIST Webbook
rinpol	691.20	NIST Webbook
rinpol	690.70	NIST Webbook
rinpol	686.00	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	691.00	NIST Webbook
rinpol	692.00	NIST Webbook
rinpol	687.10	NIST Webbook
rinpol	688.80	NIST Webbook
rinpol	690.50	NIST Webbook
rinpol	692.20	NIST Webbook
rinpol	685.00	NIST Webbook
rinpol	686.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	691.00	NIST Webbook
rinpol	693.00	NIST Webbook
rinpol	690.90	NIST Webbook
rinpol	691.20	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	696.60	NIST Webbook
rinpol	692.00	NIST Webbook
rinpol	691.60	NIST Webbook
rinpol	691.60	NIST Webbook
rinpol	697.00	NIST Webbook
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rinpol	695.00	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	692.00	NIST Webbook

rinpol	689.00	NIST Webbook
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rinpol	692.00	NIST Webbook
rinpol	694.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	689.80	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	687.10	NIST Webbook
rinpol	692.00	NIST Webbook
rinpol	692.00	NIST Webbook
rinpol	702.00	NIST Webbook
rinpol	686.00	NIST Webbook
rinpol	690.00	NIST Webbook
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rinpol	686.60	NIST Webbook
rinpol	681.78	NIST Webbook
rinpol	682.48	NIST Webbook
rinpol	690.90	NIST Webbook
rinpol	686.00	NIST Webbook
rinpol	684.12	NIST Webbook
rinpol	684.18	NIST Webbook
rinpol	683.95	NIST Webbook
rinpol	684.01	NIST Webbook
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rinpol	692.00	NIST Webbook
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rinpol	689.00	NIST Webbook
rinpol	686.00	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	702.00	NIST Webbook
rinpol	690.90	NIST Webbook

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rinpol	691.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	687.00		NIST Webbook
tb	364.65 ± 1.50	K	NIST Webbook
tb	365.00	K	KDB
tb	365.10	K	NIST Webbook
tb	364.95 ± 0.50	K	NIST Webbook
tb	364.95 ± 0.30	K	NIST Webbook
tb	364.93 ± 0.30	K	NIST Webbook
tb	365.04 ± 0.20	K	NIST Webbook
tb	365.05 ± 0.30	K	NIST Webbook
tb	365.05 ± 0.20	K	NIST Webbook
tb	364.93 ± 0.30	K	NIST Webbook
tb	365.00 ± 0.00	K	NIST Webbook
tb	365.01 ± 0.02	K	NIST Webbook
tb	365.00 ± 0.50	K	NIST Webbook
tb	365.00 ± 0.50	K	NIST Webbook
tb	364.90 ± 0.50	K	NIST Webbook
tb	364.95 ± 0.60	K	NIST Webbook
tc	553.20	K	KDB
tf	155.58 ± 0.06	K	NIST Webbook
tf	155.54 ± 0.08	K	NIST Webbook
tf	155.57 ± 0.05	K	NIST Webbook
tf	155.75 ± 0.50	K	NIST Webbook
tf	154.20 ± 2.00	K	NIST Webbook
tf	154.00 ± 2.00	K	NIST Webbook
tf	153.00 ± 3.00	K	NIST Webbook
tf	155.60	K	KDB
tt	154.10 ± 0.20	K	NIST Webbook
tt	154.20 ± 0.10	K	NIST Webbook
vc	0.362	m3/kmol	KDB
zc	0.2707370		KDB
zra	0.28		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.80	J/mol×K	499.07	Joback Method

cpg	256.86	J/mol×K	563.52	Joback Method
cpg	244.64	J/mol×K	531.30	Joback Method
cpg	173.95	J/mol×K	370.17	Joback Method
cpg	189.42	J/mol×K	402.40	Joback Method
cpg	204.20	J/mol×K	434.62	Joback Method
cpg	218.32	J/mol×K	466.85	Joback Method
dvisc	0.0003813	Pa×s	305.22	Joback Method
dvisc	0.0003124	Pa×s	337.69	Joback Method
dvisc	0.0002650	Pa×s	370.17	Joback Method
dvisc	0.0017720	Pa×s	175.31	Joback Method
dvisc	0.0010080	Pa×s	207.79	Joback Method
dvisc	0.0006678	Pa×s	240.26	Joback Method
dvisc	0.0004881	Pa×s	272.74	Joback Method
hvapt	34.00	kJ/mol	332.50	NIST Webbook
hvapt	30.86	kJ/mol	365.00	KDB
hvapt	34.20	kJ/mol	331.00	NIST Webbook
rfi	1.40941		298.15	KDB
rhoI	756.00	kg/m ³	289.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42695e+01
Coeff. B	-3.15242e+03
Coeff. C	-3.83640e+01
Temperature range (K), min.	263.83
Temperature range (K), max.	390.27

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	8.22511e+01
Coeff. B	-6.78492e+03
Coeff. C	-1.01964e+01
Coeff. D	8.36227e-06
Temperature range (K), min.	155.58
Temperature range (K), max.	553.15

Sources

KDB:	https://www.thermopedia.com/research/kdb/hcprop/showprop.php?cmpid=474
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C822504&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.thermopedia.com/research/kdb/hcprop/showprop.php?cmpid=474
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemed.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
ap:	Aniline Point
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
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
rho:	Liquid Density
rinpol:	Non-polar retention indices
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

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