Cyclopentane, 1,3-dimethyl-, trans-

Other names:	1,3-Dimethylcyclopentane, trans
	1,TRANS-3-DIMETHYLCYCLOPENTANE
	TRANS-1,3-DIMETHYLCYCLOPENTANE
	t-1,3-Dimethylcyclopentane
Inchi:	InChI=1S/C7H14/c1-6-3-4-7(2)5-6/h6-7H,3-5H2,1-2H3/t6-,7-/m0/s1
InchiKey:	XAZKFISIRYLAEE-BQBZGAKWSA-N
Formula:	C7H14
SMILES:	CC1CCC(C)C1
Mol. weight [g/mol]:	98.19
CAS:	1759-58-6

Physical Properties

Property code	Value	Unit	Source
chl	-4585.20 ± 1.10	kJ/mol	NIST Webbook
gf	36.90	kJ/mol	Joback Method
hf	-135.90 ± 1.20	kJ/mol	NIST Webbook
hfl	-170.20 ± 1.20	kJ/mol	NIST Webbook
hfus	8.89	kJ/mol	Joback Method
hvap	34.50	kJ/mol	NIST Webbook
hvap	34.30	kJ/mol	NIST Webbook
log10ws	-2.16		Crippen Method
logp	2.442		Crippen Method
mcvol	98.630	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
rinpol	686.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	680.66		NIST Webbook
rinpol	684.30		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	686.00		NIST Webbook

rinpol	687.00	NIST Webbook
rinpol	680.66	NIST Webbook
rinpol	678.00	NIST Webbook
rinpol	691.30	NIST Webbook
rinpol	682.00	NIST Webbook
rinpol	684.00	NIST Webbook
rinpol	687.00	NIST Webbook
rinpol	692.00	NIST Webbook
rinpol	686.30	NIST Webbook
rinpol	688.70	NIST Webbook
rinpol	689.10	NIST Webbook
rinpol	692.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	684.50	NIST Webbook
rinpol	686.20	NIST Webbook
rinpol	687.90	NIST Webbook
rinpol	689.70	NIST Webbook
rinpol	680.00	NIST Webbook
rinpol	684.00	NIST Webbook
rinpol	687.00	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	688.30	NIST Webbook
rinpol	688.60	NIST Webbook
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rinpol	686.00	NIST Webbook
rinpol	686.00	NIST Webbook
rinpol	687.00	NIST Webbook
rinpol	692.90	NIST Webbook
rinpol	691.60	NIST Webbook
rinpol	691.60	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	689.00	NIST Webbook
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rinpol	690.00		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	684.30		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	683.80		NIST Webbook
rinpol	678.37		NIST Webbook
rinpol	679.11		NIST Webbook
rinpol	684.80		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	680.88		NIST Webbook
rinpol	680.95		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	680.73		NIST Webbook
rinpol	680.98		NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	690.00		NIST Webbook
sl	271.54	J/mol×K	NIST Webbook
tb	363.92	K	KDB
tc	563.52	K	Joback Method
tf	139.25 ± 0.05	K	NIST Webbook
tf	130.45 ± 3.00	K	NIST Webbook
tf	130.25 ± 10.00	K	NIST Webbook
tf	139.18 ± 0.20	K	NIST Webbook
tf	138.15 ± 0.50	K	NIST Webbook
tf	139.46	K	KDB
tf	128.95 ± 4.00	K	NIST Webbook
tf	139.17 ± 0.03	K	NIST Webbook
tf	139.16 ± 0.06	K	NIST Webbook
tf	139.47 ± 0.40	K	NIST Webbook
tt	139.26 ± 0.03	K	NIST Webbook
tt	139.35 ± 0.05	K	NIST Webbook
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	231.80	J/mol×K	499.07	Joback Method
cpg	256.86	J/mol×K	563.52	Joback Method
cpl	190.87	J/mol×K	304.03	NIST Webbook
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
dvisc	0.0003813	Pa×s	305.22	Joback Method
dvisc	0.0003124	Pa×s	337.69	Joback Method
hfust	7.40	kJ/mol	139.50	NIST Webbook
hfust	7.40	kJ/mol	139.48	NIST Webbook
hfust	7.41	kJ/mol	139.50	NIST Webbook
hvapt	34.20	kJ/mol	328.00	NIST Webbook
hvapt	34.00	kJ/mol	331.00	NIST Webbook
sfust	53.04	J/mol×K	139.48	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43537e+01
Coeff. B	-3.17213e+03
Coeff. C	-3.81640e+01
Temperature range (K), min.	263.68
Temperature range (K), max.	388.98

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.09890e+01
Coeff. B	-7.10570e+03
Coeff. C	-1.15588e+01
Coeff. D	9.84000e-06
Temperature range (K), min.	139.18
Temperature range (K), max.	553.00

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/research/kdb/hcprop/showprop.php?cmpid=476
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1759586&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=476

Legend

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
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
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
sfust:	Entropy of fusion at a given temperature
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