Cyclopentane, propyl-

Other names:	1-CYCLOPENTYLPROPANE
	Cyclopentane, n-propyl-
	PROPYLCYCLOPENTANE
	n-Propylcyclopentane
Inchi:	InChI=1S/C8H16/c1-2-5-8-6-3-4-7-8/h8H,2-7H2,1H3
InchiKey:	KDIAMAVWIJYWHN-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	CCCC1CCCC1
Mol. weight [g/mol]:	112.21
CAS:	2040-96-2

Physical Properties

Property code	Value	Unit	Source
af	0.3350		KDB
ap	317.650	K	KDB
chl	-5245.60 ± 1.20	kJ/mol	NIST Webbook
chl	-5245.98 ± 0.75	kJ/mol	NIST Webbook
gf	52.63	kJ/mol	KDB
hcg	5245.65	kJ/mol	KDB
hcn	4893.565	kJ/mol	KDB
hf	-148.20	kJ/mol	KDB
hf	-148.10 ± 1.30	kJ/mol	NIST Webbook
hf	-147.60	kJ/mol	NIST Webbook
hfl	-188.70 ± 0.92	kJ/mol	NIST Webbook
hfl	-189.20 ± 1.30	kJ/mol	NIST Webbook
hfus	10.41	kJ/mol	Joback Method
hvap	41.10	kJ/mol	NIST Webbook
hvap	41.08	kJ/mol	NIST Webbook
hvap	41.10 ± 0.10	kJ/mol	NIST Webbook
hvap	41.12	kJ/mol	NIST Webbook
hvap	41.10	kJ/mol	NIST Webbook
ie	10.00 ± 0.04	eV	NIST Webbook
ie	9.34 ± 0.05	eV	NIST Webbook
log10ws	-4.74		Estimated Solubility Method
log10ws	-4.74		Aqueous Solubility Prediction Method
logp	2.977		Crippen Method

mcvol	112.720	ml/mol	McGowan Method
pc	3000.00	kPa	KDB
rinpol	830.40		NIST Webbook
rinpol	831.60		NIST Webbook
rinpol	829.40		NIST Webbook
rinpol	833.40		NIST Webbook
rinpol	829.90		NIST Webbook
rinpol	839.20		NIST Webbook
rinpol	830.10		NIST Webbook
rinpol	827.20		NIST Webbook
rinpol	833.80		NIST Webbook
rinpol	837.10		NIST Webbook
rinpol	837.30		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	830.30		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	808.20		NIST Webbook
rinpol	841.73		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	831.30		NIST Webbook

rinpol	830.00	NIST Webbook
rinpol	832.70	NIST Webbook
rinpol	827.12	NIST Webbook
rinpol	827.00	NIST Webbook
rinpol	830.60	NIST Webbook
rinpol	825.30	NIST Webbook
rinpol	825.60	NIST Webbook
rinpol	834.00	NIST Webbook
rinpol	830.00	NIST Webbook
rinpol	839.00	NIST Webbook
rinpol	828.00	NIST Webbook
rinpol	834.00	NIST Webbook
rinpol	828.00	NIST Webbook
rinpol	831.00	NIST Webbook
rinpol	832.00	NIST Webbook
rinpol	830.00	NIST Webbook
rinpol	833.00	NIST Webbook
rinpol	832.00	NIST Webbook
rinpol	830.70	NIST Webbook
rinpol	832.30	NIST Webbook
rinpol	834.50	NIST Webbook
rinpol	836.20	NIST Webbook
rinpol	837.60	NIST Webbook
rinpol	838.80	NIST Webbook
rinpol	830.00	NIST Webbook
rinpol	832.00	NIST Webbook
rinpol	834.00	NIST Webbook
rinpol	836.00	NIST Webbook
rinpol	837.00	NIST Webbook
rinpol	838.00	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	830.00	NIST Webbook
rinpol	832.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	834.00	NIST Webbook
rinpol	832.30	NIST Webbook
rinpol	836.50	NIST Webbook
rinpol	838.00	NIST Webbook
rinpol	827.00	NIST Webbook
ripol	891.00	NIST Webbook
ripol	903.00	NIST Webbook
ripol	912.00	NIST Webbook
ripol	912.00	NIST Webbook

ripol	894.00		NIST Webbook
ripol	890.60		NIST Webbook
ripol	907.10		NIST Webbook
ripol	903.00		NIST Webbook
ripol	898.00		NIST Webbook
ripol	912.00		NIST Webbook
ripol	894.00		NIST Webbook
ripol	900.00		NIST Webbook
ripol	904.00		NIST Webbook
ripol	898.00		NIST Webbook
ripol	903.00		NIST Webbook
ripol	907.00		NIST Webbook
ripol	895.00		NIST Webbook
sg	414.47	J/mol×K	NIST Webbook
sl	310.83	J/mol×K	NIST Webbook
tb	404.10	K	KDB
tc	603.00	K	KDB
tf	155.80	K	KDB
tf	156.00	K	Aqueous Solubility Prediction Method
tt	155.79 ± 0.01	K	NIST Webbook
tt	155.80 ± 0.60	K	NIST Webbook
vc	0.425	m3/kmol	KDB
zc	0.2543060		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.46	J/mol×K	590.42	Joback Method
cpg	288.65	J/mol×K	558.31	Joback Method
cpg	213.84	J/mol×K	397.72	Joback Method
cpg	230.32	J/mol×K	429.84	Joback Method
cpg	246.02	J/mol×K	461.95	Joback Method
cpg	260.95	J/mol×K	494.07	Joback Method
cpg	275.16	J/mol×K	526.19	Joback Method
cpl	216.27	J/mol×K	298.15	NIST Webbook
dvisc	0.0005131	Pa×s	328.75	Joback Method
dvisc	0.0003873	Pa×s	363.24	Joback Method
dvisc	0.0007263	Pa×s	294.27	Joback Method
dvisc	0.0011273	Pa×s	259.79	Joback Method
dvisc	0.0003069	Pa×s	397.72	Joback Method

dvisc	0.0043742	Pa×s	190.82	Joback Method
dvisc	0.0020017	Pa×s	225.30	Joback Method
hfust	10.04	kJ/mol	155.80	NIST Webbook
hfust	10.04	kJ/mol	155.80	NIST Webbook
hfust	10.03	kJ/mol	155.79	NIST Webbook
hvapt	34.70	kJ/mol	404.10	NIST Webbook
hvapt	39.20	kJ/mol	364.50	NIST Webbook
hvapt	34.11	kJ/mol	404.10	KDB
rfi	1.42389		298.15	KDB
rhol	781.00	kg/m3	289.00	KDB
sfust	64.44	J/mol×K	155.79	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	1.41315e+01
Coeff. B	-3.42008e+03
Coeff. C	-4.45910e+01
Temperature range (K), min.	291.64
Temperature range (K), max.	432.35

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.66656e+01
Coeff. B	-7.41133e+03
Coeff. C	-9.07967e+00
Coeff. D	4.79197e-06
Temperature range (K), min.	155.81
Temperature range (K), max.	603.00

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=480
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2040962&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB:	https://www.cheric.org/files/research/kdb/mol/mol480.mol

Legend

af:	Acentric Factor
ap:	Aniline Point
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
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
ripol:	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