

Cyclopentane, (1-methylethyl)-

Other names:	(1-METHYLETHYL)CYCLOPENTANE 2-CYCLOPENTYLPROPANE Cyclopentane, isopropyl- Isopropylcyclopentane Propane, 2-cyclopentyl-
Inchi:	InChI=1S/C8H16/c1-7(2)8-5-3-4-6-8/h7-8H,3-6H2,1-2H3
InchiKey:	TVSBRLGQVHJIKT-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	CC(C)C1CCCC1
Mol. weight [g/mol]:	112.21
CAS:	3875-51-2

Physical Properties

Property code	Value	Unit	Source
af	0.2400		KDB
gf	50.59	kJ/mol	Joback Method
hcg	5246.32	kJ/mol	KDB
hcn	4894.444	kJ/mol	KDB
hf	-153.25	kJ/mol	Joback Method
hfus	6.89	kJ/mol	Joback Method
hvap	39.40 ± 0.10	kJ/mol	NIST Webbook
hvap	37.90	kJ/mol	NIST Webbook
hvap	39.48	kJ/mol	NIST Webbook
log10ws	-2.58		Crippen Method
logp	2.833		Crippen Method
mvol	112.720	ml/mol	McGowan Method
pc	3000.00	kPa	KDB
rinpol	810.40		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	837.00		NIST Webbook

rinpol	812.00	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	814.00	NIST Webbook
rinpol	815.00	NIST Webbook
rinpol	818.00	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	812.20	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	812.00	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	822.00	NIST Webbook
rinpol	829.00	NIST Webbook
rinpol	810.10	NIST Webbook
rinpol	806.06	NIST Webbook
rinpol	809.20	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	812.00	NIST Webbook
rinpol	824.00	NIST Webbook
rinpol	809.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	812.00	NIST Webbook
rinpol	818.00	NIST Webbook
rinpol	812.20	NIST Webbook
rinpol	814.20	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	819.20	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	822.60	NIST Webbook
rinpol	812.00	NIST Webbook
rinpol	814.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	819.00	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	822.00	NIST Webbook
rinpol	806.00	NIST Webbook
rinpol	812.00	NIST Webbook
rinpol	808.00	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	810.10	NIST Webbook
rinpol	817.60	NIST Webbook

rinpol	829.00		NIST Webbook
rinpol	810.80		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	834.10		NIST Webbook
rinpol	832.20		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	812.10		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	818.30		NIST Webbook
tb	399.57 ± 1.00	K	NIST Webbook
tb	399.57 ± 1.00	K	NIST Webbook
tb	399.55 ± 0.50	K	NIST Webbook
tb	399.70 ± 0.40	K	NIST Webbook
tb	399.56 ± 0.02	K	NIST Webbook
tb	399.90 ± 2.00	K	NIST Webbook
tb	399.60	K	NIST Webbook
tb	399.55 ± 0.30	K	NIST Webbook
tb	399.56 ± 0.01	K	NIST Webbook
tb	399.60 ± 1.50	K	NIST Webbook
tb	399.60 ± 2.00	K	NIST Webbook
tb	399.55 ± 0.20	K	NIST Webbook
tb	399.60	K	NIST Webbook
tb	399.55 ± 0.30	K	NIST Webbook
tb	399.60	K	KDB
tb	400.10 ± 1.00	K	NIST Webbook
tc	601.00	K	KDB
tf	160.50	K	KDB
vc	0.418	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.62	J/mol×K	561.79	Joback Method
cpg	246.88	J/mol×K	463.08	Joback Method
cpg	230.72	J/mol×K	430.18	Joback Method
cpg	213.74	J/mol×K	397.28	Joback Method
cpg	262.23	J/mol×K	495.99	Joback Method
cpg	303.72	J/mol×K	594.69	Joback Method
cpg	276.80	J/mol×K	528.89	Joback Method

dvisc	0.0073344	Paxs	175.82	Joback Method
dvisc	0.0002960	Paxs	397.28	Joback Method
dvisc	0.0003843	Paxs	360.37	Joback Method
dvisc	0.0005295	Paxs	323.46	Joback Method
dvisc	0.0007925	Paxs	286.55	Joback Method
dvisc	0.0013361	Paxs	249.64	Joback Method
dvisc	0.0027005	Paxs	212.73	Joback Method
hvapt	37.90	kJ/mol	361.50	NIST Webbook
hvapt	33.56	kJ/mol	399.60	NIST Webbook
rfi	1.42350		298.15	KDB
rhol	776.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41783e+01
Coeff. B	-3.34773e+03
Coeff. C	-4.93890e+01
Temperature range (K), min.	290.39
Temperature range (K), max.	426.94

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.44288e+01
Coeff. B	-7.14690e+03
Coeff. C	-8.79687e+00
Coeff. D	4.83498e-06
Temperature range (K), min.	289.15
Temperature range (K), max.	595.38

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol481.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3875512&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.thermo.com/research/kdb/hcprop/showprop.php?cmpid=481

Legend

af:	Acentric Factor
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
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
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rho:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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