Cyclopropane

Other names:	Cyclopropnane
	TRIMETHYLENE
	Trimethylene (cyclic)
	UN 1027
Inchi:	InChI=1S/C3H6/c1-2-3-1/h1-3H2
InchiKey:	LVZWSLJZHVFIQJ-UHFFFAOYSA-N
Formula:	C3H6
SMILES:	C1CC1
Mol. weight [g/mol]:	42.08
CAS:	75-19-4

Physical Properties

Property code	Value	Unit	Source
af	0.1300		KDB
affp	750.30	kJ/mol	NIST Webbook
aigt	773.15	K	KDB
basg	722.20	kJ/mol	NIST Webbook
chg	-2091.40 ± 0.54	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
fll	2.40	% in Air	KDB
flu	10.30	% in Air	KDB
gf	104.50	kJ/mol	KDB
hf	53.34	kJ/mol	KDB
hf	53.30 ± 0.59	kJ/mol	NIST Webbook
hf	39.30	kJ/mol	NIST Webbook
hfus	0.59	kJ/mol	Joback Method
hvap	18.11	kJ/mol	NIST Webbook
hvap	17.02	kJ/mol	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	9.80 ± 0.10	eV	NIST Webbook
ie	10.30 ± 0.10	eV	NIST Webbook
ie	10.60	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	9.86 ± 0.04	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	10.06 ± 0.03	eV	NIST Webbook
ie	10.54	eV	NIST Webbook

ie	10.60 ± 0.10	eV	NIST Webbook
ie	9.93	eV	NIST Webbook
ie	9.91 ± 0.03	eV	NIST Webbook
ie	9.86	eV	NIST Webbook
log10ws	-0.97		Crippen Method
logp	1.170		Crippen Method
mcvol	42.270	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=1)		KDB
pc	5495.00 ± 20.26	kPa	NIST Webbook
pc	5540.00	kPa	KDB
pc	5579.46 ± 5.06	kPa	NIST Webbook
pc	5540.00 ± 50.00	kPa	NIST Webbook
pc	327.40 ± 1.00	kPa	NIST Webbook
rhoc	258.79 ± 2.10	kg/m3	NIST Webbook
rhoc	258.50 ± 0.29	kg/m3	NIST Webbook
rinpol	356.00		NIST Webbook
rinpol	347.00		NIST Webbook
rinpol	346.00		NIST Webbook
rinpol	345.00		NIST Webbook
rinpol	367.00		NIST Webbook
rinpol	344.00		NIST Webbook
rinpol	331.00		NIST Webbook
rinpol	346.00		NIST Webbook
rinpol	331.00		NIST Webbook
rinpol	356.00		NIST Webbook
rinpol	357.00		NIST Webbook
rinpol	351.00		NIST Webbook
rinpol	348.80		NIST Webbook
rinpol	367.00		NIST Webbook
ripol	405.00		NIST Webbook
sl	142.63	J/mol×K	NIST Webbook
tb	240.26 ± 0.30	K	NIST Webbook
tb	240.34	K	KDB
tb	240.30	K	NIST Webbook
tb	237.70 ± 1.00	K	NIST Webbook
tb	238.15 ± 2.00	K	NIST Webbook
tb	242.00 ± 4.00	K	NIST Webbook
tb	240.50 ± 0.40	K	NIST Webbook
tb	240.25 ± 1.00	K	NIST Webbook
tb	240.50	K	NIST Webbook
tc	397.80 ± 1.00	K	NIST Webbook
tc	398.00 ± 0.30	K	NIST Webbook
tc	398.30 ± 0.05	K	NIST Webbook

tc	397.80 ± 0.15	K	NIST Webbook
tc	398.00	K	KDB
tf	145.70	K	KDB
tt	145.80 ± 0.80	K	NIST Webbook
tt	145.57 ± 0.02	K	NIST Webbook
tt	145.59 ± 0.08	K	NIST Webbook
vc	0.162	m3/kmol	NIST Webbook
vc	0.162	m3/kmol	KDB
zc	0.2712100		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	59.27	J/mol×K	316.70	NIST Webbook
cpg	63.26	J/mol×K	339.60	NIST Webbook
cpg	64.27	J/mol×K	338.90	NIST Webbook
cpg	63.18	J/mol×K	333.70	NIST Webbook
cpg	55.25	J/mol×K	295.50	NIST Webbook
cpg	62.17	J/mol×K	332.80	NIST Webbook
cpg	35.38	J/mol×K	157.80	NIST Webbook
cpg	42.16	J/mol×K	220.10	NIST Webbook
cpg	42.55	J/mol×K	223.70	NIST Webbook
cpg	48.68	J/mol×K	258.70	NIST Webbook
cpg	50.63	J/mol×K	272.15	NIST Webbook
cpg	54.66	J/mol×K	291.40	NIST Webbook
cpg	60.90	J/mol×K	325.10	NIST Webbook
cpg	56.48	J/mol×K	300.48	NIST Webbook
cpg	59.29	J/mol×K	313.90	NIST Webbook
cpg	70.17	J/mol×K	368.46	NIST Webbook
cpl	81.34	J/mol×K	240.00	NIST Webbook
dvisc	0.0001853	Pa×s	257.17	Joback Method
dvisc	0.0003621	Pa×s	168.03	Joback Method
dvisc	0.0004866	Pa×s	145.75	Joback Method
dvisc	0.0002089	Pa×s	234.88	Joback Method
dvisc	0.0001676	Pa×s	279.45	Joback Method
dvisc	0.0002415	Pa×s	212.60	Joback Method
dvisc	0.0002888	Pa×s	190.32	Joback Method
hfust	5.44	kJ/mol	145.60	NIST Webbook
hfust	5.44	kJ/mol	145.60	NIST Webbook
hfust	5.44	kJ/mol	145.57	NIST Webbook

hsubt	29.20	kJ/mol	145.00	NIST Webbook
hsubt	28.20	kJ/mol	128.00	NIST Webbook
hvapt	20.40	kJ/mol	378.00	NIST Webbook
hvapt	20.05	kJ/mol	240.30	NIST Webbook
hvapt	19.90	kJ/mol	268.50	NIST Webbook
hvapt	21.10	kJ/mol	212.00	NIST Webbook
hvapt	21.80	kJ/mol	210.00	NIST Webbook
hvapt	20.05	kJ/mol	240.34	NIST Webbook
hvapt	19.90	kJ/mol	328.00	NIST Webbook
hvapt	20.30	kJ/mol	213.50	NIST Webbook
hvapt	20.04	kJ/mol	240.30	KDB
pvap	344.10	kPa	273.15	Isothermal vapour + liquid equilibrium measurements and correlation for the pentafluoroethane + cyclopropane and the cyclopropane + 1,1,1,2-tetrafluoroethane binary systems
pvap	344.70	kPa	273.15	Isothermal vapour + liquid equilibrium measurements and correlation for the pentafluoroethane + cyclopropane and the cyclopropane + 1,1,1,2-tetrafluoroethane binary systems
pvap	631.70	kPa	293.15	Isothermal vapour + liquid equilibrium measurements and correlation for the pentafluoroethane + cyclopropane and the cyclopropane + 1,1,1,2-tetrafluoroethane binary systems
pvap	632.20	kPa	293.15	Isothermal vapour + liquid equilibrium measurements and correlation for the pentafluoroethane + cyclopropane and the cyclopropane + 1,1,1,2-tetrafluoroethane binary systems

pvap	171.30	kPa	253.15	Isothermal vapour + liquid equilibrium measurements and correlation for the pentafluoroethane + cyclopropane and the cyclopropane + 1,1,1,2-tetrafluoroethane binary systems
pvap	171.20	kPa	253.15	Isothermal vapour + liquid equilibrium measurements and correlation for the pentafluoroethane + cyclopropane and the cyclopropane + 1,1,1,2-tetrafluoroethane binary systems
rhol	631.00	kg/m3	288.70	KDB
sfust	37.39	J/mol×K	145.57	NIST Webbook
srf	0.01	N/m	298.20	KDB
svapt	83.44	J/mol×K	240.34	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43518e+01
Coeff. B	-2.11825e+03
Coeff. C	-2.23740e+01
Temperature range (K), min.	172.99
Temperature range (K), max.	398.30

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.36950e+01
Coeff. B	-3.98970e+03
Coeff. C	-7.89343e+00
Coeff. D	1.38201e-05
Temperature range (K), min.	145.59

Temperature range (K), max.	397.91

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75194&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Isothermal vapour + liquid equilibrium measurements and correlation for the pentafluoroethane + cyclopropane and 1,1,1,2-tetrafluoroethane + cyclopropane systems:	https://www.doi.org/10.1016/j.fluid.2006.10.023
Solubilities of isobutane and cyclopropane in ionic liquids:	https://www.doi.org/10.1016/j.jct.2015.04.013
KDB:	https://www.cheric.org/files/research/kdb/mol/mol446.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=446

Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation 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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
svapt:	Entropy of vaporization at a given temperature
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