Cyclobutane

Other names: TETRAMETHYLENE
UN 2601
Inchi: InChI=1S/C4H8/c1-2-4-3-1/h1-4H2
InchiKey: PMPVIKIVABFJJI-UHFFFAOYSA-N
Formula: C4H8
SMILES: C1CCC1
Mol. weight [g/mol]: 56.11
CAS: 287-23-0

Physical Properties

Property code	Value	Unit	Source
af	0.1810		KDB
chl	-2720.40 ± 0.50	kJ/mol	NIST Webbook
chl	-2720.50 ± 0.40	kJ/mol	NIST Webbook
gf	110.10	kJ/mol	KDB
hcg	2720.56	kJ/mol	KDB
hcn	2544.541	kJ/mol	KDB
hf	26.67	kJ/mol	KDB
hfus	1.08	kJ/mol	Joback Method
hvap	23.30 ± 0.40	kJ/mol	NIST Webbook
hvap	23.20	kJ/mol	NIST Webbook
hvap	23.92	kJ/mol	NIST Webbook
ie	10.70 ± 0.10	eV	NIST Webbook
ie	10.06	eV	NIST Webbook
ie	10.30	eV	NIST Webbook
ie	9.92 ± 0.05	eV	NIST Webbook
ie	9.60 ± 0.10	eV	NIST Webbook
ie	10.70 ± 0.10	eV	NIST Webbook
ie	9.80 ± 0.10	eV	NIST Webbook
ie	9.82 ± 0.05	eV	NIST Webbook
log10ws	-1.39		Crippen Method
logp	1.560		Crippen Method
mcvol	56.360	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=1)		KDB
pc	4980.00	kPa	KDB
rinpol	462.00		NIST Webbook

rinpol	467.00		NIST Webbook
rinpol	465.00		NIST Webbook
rinpol	464.00		NIST Webbook
sl	175.15	J/mol×K	NIST Webbook
tb	285.73 ± 0.40	K	NIST Webbook
tb	284.45 ± 1.00	K	NIST Webbook
tb	284.40 ± 1.00	K	NIST Webbook
tb	285.70 ± 0.60	K	NIST Webbook
tb	284.65 ± 2.00	K	NIST Webbook
tb	277.90 ± 8.00	K	NIST Webbook
tb	285.70	K	KDB
tb	285.70	K	NIST Webbook
tb	285.70	K	NIST Webbook
tb	284.00 ± 2.00	K	NIST Webbook
tc	460.00	K	KDB
tf	183.00 ± 1.00	K	NIST Webbook
tf	273.14 ± 3.00	K	NIST Webbook
tf	193.00 ± 3.00	K	NIST Webbook
tf	182.48	K	KDB
tt	182.07 ± 0.20	K	NIST Webbook
tt	182.45 ± 0.10	K	NIST Webbook
tt	182.56 ± 0.20	K	NIST Webbook
tt	182.07 ± 0.30	K	NIST Webbook
tt	182.45 ± 0.07	K	NIST Webbook
tt	181.94 ± 0.30	K	NIST Webbook
tt	182.42 ± 0.07	K	NIST Webbook
tt	183.00 ± 3.00	K	NIST Webbook
tt	181.94 ± 0.30	K	NIST Webbook
tt	182.42 ± 0.10	K	NIST Webbook
tt	182.79 ± 0.10	K	NIST Webbook
tt	182.56 ± 0.20	K	NIST Webbook
vc	0.210	m3/kmol	KDB
zc	0.2734350		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	71.17	J/mol×K	306.60	Joback Method
cpg	90.62	J/mol×K	368.97	Joback Method
cpg	99.53	J/mol×K	400.16	Joback Method
cpg	107.93	J/mol×K	431.35	Joback Method

cpg	115.85	J/mol×K	462.53	Joback Method
cpg	123.30	J/mol×K	493.72	Joback Method
cpg	81.17	J/mol×K	337.79	Joback Method
cpl	106.32	J/mol×K	285.00	NIST Webbook
dvisc	0.0003735	Pa×s	255.57	Joback Method
dvisc	0.0004914	Pa×s	230.05	Joback Method
dvisc	0.0006924	Pa×s	204.53	Joback Method
dvisc	0.0010758	Pa×s	179.02	Joback Method
dvisc	0.0019353	Pa×s	153.50	Joback Method
dvisc	0.0002474	Pa×s	306.60	Joback Method
dvisc	0.0002984	Pa×s	281.08	Joback Method
hfust	1.09	kJ/mol	182.40	NIST Webbook
hfust	5.71	kJ/mol	145.70	NIST Webbook
hfust	1.09	kJ/mol	182.40	NIST Webbook
hsubt	36.40	kJ/mol	145.00	NIST Webbook
hvapt	25.20	kJ/mol	251.00	NIST Webbook
hvapt	25.20	kJ/mol	242.50	NIST Webbook
hvapt	24.19	kJ/mol	285.70	NIST Webbook
hvapt	24.19	kJ/mol	285.66	NIST Webbook
hvapt	24.18	kJ/mol	285.70	KDB
hvapt	5.78	kJ/mol	559.00	NIST Webbook
rfi	1.36200		298.15	KDB
rhol	694.00	kg/m3	293.00	KDB
sfust	39.17	J/mol×K	145.70	NIST Webbook
sfust	5.96	J/mol×K	182.40	NIST Webbook
svapt	84.67	J/mol×K	285.66	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45761e+01
Coeff. B	-2.59227e+03
Coeff. C	-2.36740e+01
Temperature range (K), min.	182.48
Temperature range (K), max.	303.48

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.98565e+01
Coeff. B	-4.57855e+03
Coeff. C	-7.06594e+00
Coeff. D	9.11328e-06
Temperature range (K), min.	182.48
Temperature range (K), max.	460.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C287230&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=448
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=448

Legend

af:	Acentric Factor
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
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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
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