Cyclobutane, methylene-

Other names: Methylenecyclobutane
Inchi: InChI=1S/C5H8/c1-5-3-2-4-5/h1-4H2
InchiKey: QIRVGKYPAOQVNP-UHFFFAOYSA-N
Formula: C5H8
SMILES: C=C1CCC1
Mol. weight [g/mol]: 68.12
CAS: 1120-56-5

Physical Properties

Property code	Value	Unit	Source
chl	-3204.70 ± 0.50	kJ/mol	NIST Webbook
gf	100.66	kJ/mol	Joback Method
hf	121.50 ± 0.71	kJ/mol	NIST Webbook
hf	106.00	kJ/mol	NIST Webbook
hfl	93.85 ± 0.59	kJ/mol	NIST Webbook
hfus	2.51	kJ/mol	Joback Method
hvap	27.70 ± 0.40	kJ/mol	NIST Webbook
hvap	27.70 ± 0.42	kJ/mol	NIST Webbook
hvap	27.70	kJ/mol	NIST Webbook
ie	9.19 ± 0.02	eV	NIST Webbook
ie	9.35	eV	NIST Webbook
ie	9.16 ± 0.02	eV	NIST Webbook
ie	9.12	eV	NIST Webbook
ie	9.14 ± 0.08	eV	NIST Webbook
log10ws	-1.66		Crippen Method
logp	1.727		Crippen Method
mcvol	66.150	ml/mol	McGowan Method
pc	4498.26	kPa	Joback Method
rinpol	539.00		NIST Webbook
rinpol	535.00		NIST Webbook
rinpol	539.00		NIST Webbook
rinpol	537.00		NIST Webbook
rinpol	536.00		NIST Webbook
rinpol	534.00		NIST Webbook
rinpol	546.00		NIST Webbook
rinpol	535.00		NIST Webbook
rinpol	536.00		NIST Webbook

rinpol	536.00		NIST Webbook
sg	298.90 ± 1.00	J/mol×K	NIST Webbook
sl	210.60	J/mol×K	NIST Webbook
sl	210.60	J/mol×K	NIST Webbook
sl	210.20	J/mol×K	NIST Webbook
sl	210.60	J/mol×K	NIST Webbook
tb	315.37 ± 0.10	K	NIST Webbook
tb	308.30 ± 5.00	K	NIST Webbook
tb	314.90 ± 1.00	K	NIST Webbook
tb	315.00 ± 2.00	K	NIST Webbook
tb	315.00 ± 2.00	K	NIST Webbook
tb	315.00 ± 3.00	K	NIST Webbook
tb	315.40	K	NIST Webbook
tb	315.00 ± 4.00	K	NIST Webbook
tb	315.00 ± 4.00	K	NIST Webbook
tb	315.35 ± 0.30	K	NIST Webbook
tc	517.90	K	Joback Method
tf	138.47 ± 0.20	K	NIST Webbook
tt	138.53 ± 0.01	K	NIST Webbook
tt	138.62 ± 0.01	K	NIST Webbook
vc	0.249	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.16	J/mol×K	423.27	Joback Method
cpg	131.32	J/mol×K	454.81	Joback Method
cpg	139.03	J/mol×K	486.36	Joback Method
cpg	95.78	J/mol×K	328.64	Joback Method
cpg	105.41	J/mol×K	360.18	Joback Method
cpg	114.54	J/mol×K	391.73	Joback Method
cpg	146.31	J/mol×K	517.90	Joback Method
cpl	131.10	J/mol×K	298.15	NIST Webbook
cpl	133.60	J/mol×K	298.15	NIST Webbook
cpl	133.60	J/mol×K	298.15	NIST Webbook
cpl	133.60	J/mol×K	298.15	NIST Webbook
dvisc	0.0011307	Pa×s	178.45	Joback Method
dvisc	0.0005588	Pa×s	228.51	Joback Method
dvisc	0.0004361	Pa×s	253.54	Joback Method
dvisc	0.0003558	Pa×s	278.58	Joback Method
dvisc	0.0003002	Pa×s	303.61	Joback Method

dvisc	0.0002599	Pa×s	328.64	Joback Method
dvisc	0.0007612	Pa×s	203.48	Joback Method
hfust	5.76	kJ/mol	138.62	NIST Webbook
hfust	5.86	kJ/mol	138.50	NIST Webbook
hfust	5.75	kJ/mol	138.62	NIST Webbook
hfust	5.86	kJ/mol	138.50	NIST Webbook
hfust	5.75	kJ/mol	138.62	NIST Webbook
hvapt	29.10	kJ/mol	299.00	NIST Webbook
hvapt	26.10	kJ/mol	303.00	NIST Webbook
sfust	41.60	J/mol×K	138.62	NIST Webbook
sfust	41.60	J/mol×K	138.62	NIST Webbook
sfust	41.60	J/mol×K	138.62	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	315.20	K	99.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38886e+01
Coeff. B	-2.53404e+03
Coeff. C	-4.19990e+01
Temperature range (K), min.	228.31
Temperature range (K), max.	337.44

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1120565&Units=SI

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
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
rinpol:	Non-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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume