Cyclobutane, methyl-

Other names: 1-METHYLCYCLOBUTANE
Methylcyclobutane
Inchi: InChI=1S/C5H10/c1-5-3-2-4-5/h5H,2-4H2,1H3
InchiKey: BDJAEZRIGNCQBZ-UHFFFAOYSA-N
Formula: C5H10
SMILES: CC1CCC1
Mol. weight [g/mol]: 70.13
CAS: 598-61-8

Physical Properties

Property code	Value	Unit	Source
chg	-3352.00 ± 1.30	kJ/mol	NIST Webbook
gf	39.87	kJ/mol	Joback Method
hf	-79.89	kJ/mol	Joback Method
hfus	4.74	kJ/mol	Joback Method
hvap	26.81	kJ/mol	Joback Method
ie	9.60	eV	NIST Webbook
ie	9.64 ± 0.05	eV	NIST Webbook
log10ws	-1.57		Crippen Method
logp	1.806		Crippen Method
mcvol	70.450	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpol	513.00		NIST Webbook
rinpol	538.90		NIST Webbook
rinpol	535.50		NIST Webbook
tb	324.81	K	Joback Method
tc	511.38	K	Joback Method
tf	160.53	K	Joback Method
vc	0.265	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.51	J/mol×K	480.29	Joback Method

cpg	147.05	J/mol×K	449.19	Joback Method
cpg	137.08	J/mol×K	418.10	Joback Method
cpg	126.59	J/mol×K	387.00	Joback Method
cpg	115.54	J/mol×K	355.91	Joback Method
cpg	103.91	J/mol×K	324.81	Joback Method
cpg	165.48	J/mol×K	511.38	Joback Method
dvisc	0.0010796	Pa×s	160.53	Joback Method
dvisc	0.0002389	Pa×s	324.81	Joback Method
dvisc	0.0002736	Pa×s	297.43	Joback Method
dvisc	0.0003221	Pa×s	270.05	Joback Method
dvisc	0.0003934	Pa×s	242.67	Joback Method
dvisc	0.0005056	Pa×s	215.29	Joback Method
dvisc	0.0006991	Pa×s	187.91	Joback Method
hfust	5.76	kJ/mol	138.60	NIST Webbook
hfust	5.76	kJ/mol	138.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37385e+01
Coeff. B	-2.61286e+03
Coeff. C	-2.55090e+01
Temperature range (K), min.	219.76
Temperature range (K), max.	335.56

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C598618&Units=SI

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol453.mol

Legend

chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
hvap:	Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume