Cyclopropane, 1,1-dimethyl-

Other names:	1,1-Dimethylcyclopropane
	GEM-DIMETHYLCYCLOROPANE
	Gem-Dimethylcyclopropane
Inchi:	InChI=1S/C5H10/c1-5(2)3-4-5/h3-4H2,1-2H3
InchiKey:	PBIJFSCPEFQXBB-UHFFFAOYSA-N
Formula:	C5H10
SMILES:	CC1(C)CC1
Mol. weight [g/mol]:	70.13
CAS:	1630-94-0

Physical Properties

Property code	Value	Unit	Source
chl	-3363.40 ± 0.71	kJ/mol	NIST Webbook
gf	46.48	kJ/mol	Joback Method
hf	-8.20 ± 1.20	kJ/mol	NIST Webbook
hfl	-33.30 ± 0.79	kJ/mol	NIST Webbook
hfus	0.54	kJ/mol	Joback Method
hvap	25.10 ± 0.80	kJ/mol	NIST Webbook
hvap	25.00 ± 0.80	kJ/mol	NIST Webbook
hvap	25.10	kJ/mol	NIST Webbook
ie	9.08	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
ie	8.98 ± 0.05	eV	NIST Webbook
ie	9.76 ± 0.02	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
log10ws	-1.57		Crippen Method
logp	1.806		Crippen Method
mcvol	70.450	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
rinpol	460.00		NIST Webbook
rinpol	460.00		NIST Webbook
rinpol	460.00		NIST Webbook
rinpol	459.00		NIST Webbook
rinpol	458.80		NIST Webbook
rinpol	459.00		NIST Webbook
tb	320.78	K	Joback Method
tc	507.71	K	Joback Method

tf	187.95	K	Joback Method
vc	0.271	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	105.46	J/mol×K	320.78	Joback Method
cpg	117.91	J/mol×K	351.93	Joback Method
cpg	129.33	J/mol×K	383.09	Joback Method
cpg	139.80	J/mol×K	414.24	Joback Method
cpg	149.40	J/mol×K	445.40	Joback Method
cpg	158.22	J/mol×K	476.55	Joback Method
cpg	166.32	J/mol×K	507.71	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42059e+01
Coeff. B	-2.46430e+03
Coeff. C	-3.79700e+01
Temperature range (K), min.	215.02
Temperature range (K), max.	315.03

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol450.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1630940&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
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