Cyclobutene

Inchi: InChI=1S/C4H6/c1-2-4-3-1/h1-2H,3-4H2
InchiKey: CFBGXYDUODCMNS-UHFFFAOYSA-N
Formula: C4H6
SMILES: C1=CCC1
Mol. weight [g/mol]: 54.09
CAS: 822-35-5

Physical Properties

Property code	Value	Unit	Source
af	0.1890		KDB
affp	784.40	kJ/mol	NIST Webbook
basg	753.60	kJ/mol	NIST Webbook
chg	-2588.20 ± 1.50	kJ/mol	NIST Webbook
gf	69.12	kJ/mol	Joback Method
hf	157.00 ± 2.00	kJ/mol	NIST Webbook
hfus	2.30	kJ/mol	Joback Method
hvap	25.18	kJ/mol	Joback Method
ie	9.43	eV	NIST Webbook
ie	9.43 ± 0.03	eV	NIST Webbook
ie	9.59	eV	NIST Webbook
ie	9.43	eV	NIST Webbook
ie	9.43 ± 0.02	eV	NIST Webbook
ie	9.43 ± 0.02	eV	NIST Webbook
log10ws	-1.25		Crippen Method
logp	1.336		Crippen Method
mcvol	52.060	ml/mol	McGowan Method
pc	5270.00	kPa	KDB
rinpol	433.00		NIST Webbook
rinpol	433.00		NIST Webbook
rinpol	434.00		NIST Webbook
rinpol	432.00		NIST Webbook
tb	275.20	K	NIST Webbook
tb	275.80	K	KDB
tc	446.30	K	KDB
tf	154.00	K	KDB
vc	0.196	m3/kmol	KDB
zc	0.2776480		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	62.86	J/mol×K	305.76	Joback Method
cpg	71.52	J/mol×K	337.29	Joback Method
cpg	79.64	J/mol×K	368.81	Joback Method
cpg	87.25	J/mol×K	400.34	Joback Method
cpg	94.37	J/mol×K	431.86	Joback Method
cpg	101.04	J/mol×K	463.39	Joback Method
cpg	107.27	J/mol×K	494.92	Joback Method
dvisc	0.0007300	Pa×s	179.51	Joback Method
dvisc	0.0011908	Pa×s	154.26	Joback Method
dvisc	0.0005050	Pa×s	204.76	Joback Method
dvisc	0.0003788	Pa×s	230.01	Joback Method
dvisc	0.0003007	Pa×s	255.26	Joback Method
dvisc	0.0002489	Pa×s	280.51	Joback Method
dvisc	0.0002125	Pa×s	305.76	Joback Method
hvapt	25.81	kJ/mol	275.80	KDB
hvapt	24.70	kJ/mol	240.50	NIST Webbook
hvapt	24.60	kJ/mol	235.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45824e+01
Coeff. B	-2.55142e+03
Coeff. C	-1.91380e+01
Temperature range (K), min.	196.15
Temperature range (K), max.	295.08

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.11908e+01

Coeff. B	-4.13962e+03
Coeff. C	-5.72351e+00
Coeff. D	7.96917e-06
Temperature range (K), min.	196.15
Temperature range (K), max.	446.33

Sources

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/mol607.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C822355&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=607
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
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
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility