Cyclobutanol

Other names:	Cyclobutyl alcohol
	Cyclobutyl hydroxide
Inchi:	InChI=1S/C4H8O/c5-4-2-1-3-4/h4-5H,1-3H2
InchiKey:	KTHXBEHDVMTNOH-UHFFFAOYSA-N
Formula:	C4H8O
SMILES:	OC1CCC1
Mol. weight [g/mol]:	72.11
CAS:	2919-23-5

Physical Properties

Property code	Value	Unit	Source
affp	792.00 ± 6.00	kJ/mol	NIST Webbook
chl	-2518.20 ± 0.67	kJ/mol	NIST Webbook
gf	-105.37	kJ/mol	Joback Method
hf	-145.00	kJ/mol	NIST Webbook
hfl	-199.00	kJ/mol	NIST Webbook
hfus	7.91	kJ/mol	Heat capacities of selected cycloalcohols
hvap	54.40	kJ/mol	NIST Webbook
hvap	54.00	kJ/mol	NIST Webbook
ie	9.56 ± 0.02	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
log10ws	-0.77		Crippen Method
logp	0.531		Crippen Method
mcvol	62.230	ml/mol	McGowan Method
pc	5446.55	kPa	Joback Method
tb	396.00 ± 6.00	K	NIST Webbook
tb	398.00 ± 3.00	K	NIST Webbook
tc	577.28	K	Joback Method
tf	210.08	K	Joback Method
vc	0.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.54	J/mol×K	577.28	Joback Method
cpg	154.79	J/mol×K	546.75	Joback Method
cpg	147.64	J/mol×K	516.22	Joback Method
cpg	140.09	J/mol×K	485.69	Joback Method
cpg	132.11	J/mol×K	455.17	Joback Method
cpg	123.68	J/mol×K	424.64	Joback Method
cpg	114.78	J/mol×K	394.11	Joback Method
dvisc	0.0447052	Pa×s	210.08	Joback Method
dvisc	0.0004160	Pa×s	394.11	Joback Method
dvisc	0.0006529	Pa×s	363.44	Joback Method
dvisc	0.0011132	Pa×s	332.77	Joback Method
dvisc	0.0021154	Pa×s	302.10	Joback Method
dvisc	0.0046477	Pa×s	271.42	Joback Method
dvisc	0.0124788	Pa×s	240.75	Joback Method
hfust	8.53	kJ/mol	228.40	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	396.20	K	97.70	NIST Webbook

Sources

Heat capacities of selected cycloalcohols: https://www.doi.org/10.1016/j.tca.2014.10.002

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1219.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2919235&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
chl:	Standard liquid 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
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume