

Cyclopropanecarboxylic acid

Other names:	Carboxycyclopropane Cyclopropionic acid Cyclopropylcarboxylic acid Cyclopropylmethanoic acid Cyclpropanecarboxylic acid
Inchi:	InChI=1S/C4H6O2/c5-4(6)3-1-2-3/h3H,1-2H2,(H,5,6)
InchiKey:	YMGUBTXCNDTFJI-UHFFFAOYSA-N
Formula:	C4H6O2
SMILES:	O=C(O)C1CC1
Mol. weight [g/mol]:	86.09
CAS:	1759-53-1

Physical Properties

Property code	Value	Unit	Source
affp	821.40	kJ/mol	NIST Webbook
basg	790.40	kJ/mol	NIST Webbook
chl	-2035.00	kJ/mol	NIST Webbook
chl	-2007.00	kJ/mol	NIST Webbook
gf	-222.19	kJ/mol	Joback Method
hf	-317.90	kJ/mol	Joback Method
hfus	9.94	kJ/mol	Joback Method
hvap	47.84	kJ/mol	Joback Method
ie	10.64	eV	NIST Webbook
log10ws	-0.25		Crippen Method
logp	0.481		Crippen Method
mcvol	63.800	ml/mol	McGowan Method
pc	5765.39	kPa	Joback Method
rinpol	900.00		NIST Webbook
ripol	1811.00		NIST Webbook
ripol	1811.00		NIST Webbook
tb	456.00 ± 1.00	K	NIST Webbook
tb	456.20	K	NIST Webbook
tc	631.68	K	Joback Method
tf	263.53	K	Joback Method
vc	0.241	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.53	J/mol×K	537.70	Joback Method
cpg	144.02	J/mol×K	506.37	Joback Method
cpg	137.08	J/mol×K	475.04	Joback Method
cpg	129.68	J/mol×K	443.71	Joback Method
cpg	167.74	J/mol×K	631.68	Joback Method
cpg	162.37	J/mol×K	600.35	Joback Method
cpg	156.64	J/mol×K	569.02	Joback Method
dvisc	0.0033060	Pa×s	298.15	Densities and Viscosities of Binary Mixtures of Cyclopropanecarboxylic Acid with Methanol, Ethanol, Propan-1-ol, and Butan-1-ol at Different Temperatures
dvisc	0.0014590	Pa×s	338.15	Densities and Viscosities of Binary Mixtures of Cyclopropanecarboxylic Acid with Methanol, Ethanol, Propan-1-ol, and Butan-1-ol at Different Temperatures
dvisc	0.0017390	Pa×s	328.15	Densities and Viscosities of Binary Mixtures of Cyclopropanecarboxylic Acid with Methanol, Ethanol, Propan-1-ol, and Butan-1-ol at Different Temperatures

dvisc	0.0021020	Pa×s	318.15	Densities and Viscosities of Binary Mixtures of Cyclopropanecarboxylic Acid with Methanol, Ethanol, Propan-1-ol, and Butan-1-ol at Different Temperatures
dvisc	0.0026030	Pa×s	308.15	Densities and Viscosities of Binary Mixtures of Cyclopropanecarboxylic Acid with Methanol, Ethanol, Propan-1-ol, and Butan-1-ol at Different Temperatures
hvapt	52.40 ± 0.20	kJ/mol	415.00	NIST Webbook
hvapt	55.70 ± 0.20	kJ/mol	415.00	NIST Webbook
hvapt	58.90 ± 0.30	kJ/mol	415.00	NIST Webbook
hvapt	48.80 ± 0.40	kJ/mol	415.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56785e+01
Coeff. B	-4.29345e+03
Coeff. C	-6.79600e+01
Temperature range (K), min.	346.92
Temperature range (K), max.	482.10

Sources

Densities and Viscosities of Binary Mixtures of Cyclopropanecarboxylic Acid with Methanol, Ethanol, Propan-1-ol, and Butan-1-ol at Different Temperatures.

NIST Webbook:

<https://www.doi.org/10.1021/je800930v>

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

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1759531&Units=SI>

**The Yaws Handbook of Vapor
Pressure:
Crippen Method:**
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<http://pubs.acs.org/doi/abs/10.1021/ci990307l>
https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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