

# Propanoic acid, 2-oxo-

Other names:	2-Oxopropanoic acid
	2-Oxopropionic acid
	Acetylformic acid
	BTS
	CH3COCO <sup>OH</sup>
	Pyroracemic Acid
	Pyruvic acid
	«alpha»-Ketopropionic acid
	Â«alphaÂ»-Ketopropionic acid
	InChI=1S/C3H4O3/c1-2(4)3(5)6/h1H3,(H,5,6)
Inchi:	
InchiKey:	LCTONWCANYUPML-UHFFFAOYSA-N
Formula:	C3H4O3
SMILES:	CC(=O)C(=O)O
Mol. weight [g/mol]:	88.06
CAS:	127-17-3

## Physical Properties

Property code	Value	Unit	Source
chl	-1165.30	kJ/mol	NIST Webbook
chs	-1166.40	kJ/mol	NIST Webbook
gf	-420.28	kJ/mol	Joback Method
hf	-482.64	kJ/mol	Joback Method
hfus	10.81	kJ/mol	Joback Method
hvap	52.44	kJ/mol	Joback Method
ie	10.42	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
log10ws	0.54		Crippen Method
logp	-0.340		Crippen Method
mcvol	62.140	ml/mol	McGowan Method
pc	6027.93	kPa	Joback Method
rinpol	1249.00		NIST Webbook
tb	438.20	K	NIST Webbook
tc	654.04	K	Joback Method
tf	284.25	K	Joback Method
vc	0.234	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.70	J/molxK	467.96	Joback Method
cpg	126.81	J/molxK	529.99	Joback Method
cpg	131.05	J/molxK	561.00	Joback Method
cpg	135.09	J/molxK	592.01	Joback Method
cpg	138.94	J/molxK	623.03	Joback Method
cpg	142.58	J/molxK	654.04	Joback Method
cpg	122.36	J/molxK	498.97	Joback Method
dvisc	0.0050326	Paxs	314.87	Joback Method
dvisc	0.0022852	Paxs	345.49	Joback Method
dvisc	0.0011800	Paxs	376.11	Joback Method
dvisc	0.0006731	Paxs	406.72	Joback Method
dvisc	0.0004153	Paxs	437.34	Joback Method
dvisc	0.0131377	Paxs	284.25	Joback Method
dvisc	0.0002730	Paxs	467.96	Joback Method
hvapt	51.40	kJ/mol	366.00	NIST Webbook
pvap	0.51	kPa	318.30	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	1.09	kPa	330.80	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.80	kPa	325.80	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.60	kPa	320.90	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.60	kPa	320.90	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	1.27	kPa	333.20	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.45	kPa	316.80	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.43	kPa	315.90	Thermodynamic properties of pyruvic acid and its methyl ester

pvap	0.38	kPa	313.30	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.38	kPa	313.30	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.29	kPa	308.20	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	1.52	kPa	336.40	Thermodynamic properties of pyruvic acid and its methyl ester

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	3.45292e+01
Coeff. B	-1.05077e+04
Coeff. C	-2.48320e+01
Temperature range (K), min.	331.70
Temperature range (K), max.	384.47

## Sources

Liquid liquid equilibria for the system (water + carboxylic acid + chloroform): Phase equilibria for ternary liquid systems of (water + carboxylic acid or alcohol + Phenol) at T = 293.15 K: Crippen Method: modelling considerations: Crippen Method:	<a href="https://www.doi.org/10.1016/j.fluid.2006.02.017">https://www.doi.org/10.1016/j.fluid.2006.02.017</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C127173&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C127173&amp;Units=SI</a>
Thermodynamic properties of pyruvic acid and its methyl ester: Joback Method:	<a href="https://www.doi.org/10.1016/j.tca.2018.05.009">https://www.doi.org/10.1016/j.tca.2018.05.009</a> <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
Phase equilibria of ternary systems (water + pyruvic acid + high boiling alcohol): The Yaws Handbook of Vapor Pressure and Boiling Point Data: Prediction of extraction:	<a href="https://www.doi.org/10.1016/j.jct.2012.06.019">https://www.doi.org/10.1016/j.jct.2012.06.019</a> <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>

# Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>chs:</b>	Standard solid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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