2-Propanone, 1-hydroxy-

Other names:	1-Hydroxypropan-2-one
	1-hydroxy-2-propanone
	Acetone alcohol
	Acetylcarbinol
	CH3C(O)CH2OH
	Hydroxypropan-2-one
	Methanol, acetyl-
	acetol
	hydroxyacetone
	hydroxyacetone (acetol)
	hydroxypropanone
Inchi:	InChI=1S/C3H6O2/c1-3(5)2-4/h4H,2H2,1H3
InchiKey:	XLSMFKSTNGKWQX-UHFFFAOYSA-N
Formula:	C3H6O2
SMILES:	CC(=O)CO
Mol. weight [g/mol]:	74.08
CAS:	116-09-6

Physical Properties

Property code	Value	Unit	Source
gf	-291.36	kJ/mol	Joback Method
hf	-370.06	kJ/mol	Joback Method
hfus	9.21	kJ/mol	Joback Method
hvap	45.70	kJ/mol	Joback Method
ie	10.00 ± 0.10	eV	NIST Webbook
log10ws	0.38		Crippen Method
logp	-0.432		Crippen Method
mcvol	60.570	ml/mol	McGowan Method
pc	5478.85	kPa	Joback Method
rinpol	625.00		NIST Webbook
rinpol	652.00		NIST Webbook
rinpol	652.00		NIST Webbook
rinpol	662.00		NIST Webbook
rinpol	666.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	625.00		NIST Webbook

rinpol	655.00	NIST Webbook
rinpol	694.00	NIST Webbook
rinpol	632.00	NIST Webbook
rinpol	631.00	NIST Webbook
rinpol	668.00	NIST Webbook
rinpol	668.00	NIST Webbook
rinpol	620.00	NIST Webbook
rinpol	660.00	NIST Webbook
rinpol	625.00	NIST Webbook
rinpol	640.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	713.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	658.00	NIST Webbook
rinpol	658.00	NIST Webbook
rinpol	674.00	NIST Webbook
rinpol	663.00	NIST Webbook
rinpol	666.00	NIST Webbook
rinpol	664.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	674.00	NIST Webbook
rinpol	655.00	NIST Webbook
rinpol	668.00	NIST Webbook
ripol	1305.00	NIST Webbook
ripol	1306.00	NIST Webbook
ripol	1323.00	NIST Webbook
ripol	1298.00	NIST Webbook
ripol	1266.00	NIST Webbook
ripol	1277.00	NIST Webbook
ripol	1284.00	NIST Webbook
ripol	1290.00	NIST Webbook
ripol	1275.00	NIST Webbook
ripol	1318.00	NIST Webbook
ripol	1318.00	NIST Webbook
ripol	1303.00	NIST Webbook
ripol	1296.00	NIST Webbook
ripol	1303.00	NIST Webbook
ripol	1295.00	NIST Webbook
ripol	1304.00	NIST Webbook
ripol	1317.00	NIST Webbook
ripol	1289.00	NIST Webbook
ripol	1278.00	NIST Webbook
ripol	1304.00	NIST Webbook
ripol	1303.00	NIST Webbook

ripol	1321.00	NIST Webbook
ripol	1310.00	NIST Webbook
ripol	1315.00	NIST Webbook
ripol	1326.00	NIST Webbook
ripol	1321.00	NIST Webbook
ripol	1319.00	NIST Webbook
ripol	1312.00	NIST Webbook
ripol	1306.00	NIST Webbook
ripol	1298.00	NIST Webbook
ripol	1274.00	NIST Webbook
ripol	1297.00	NIST Webbook
ripol	1340.00	NIST Webbook
ripol	1315.00	NIST Webbook
ripol	1318.00	NIST Webbook
ripol	1307.00	NIST Webbook
ripol	1313.00	NIST Webbook
ripol	1295.00	NIST Webbook
ripol	1296.00	NIST Webbook
ripol	1315.00	NIST Webbook
ripol	1326.00	NIST Webbook
ripol	1268.00	NIST Webbook
ripol	1323.00	NIST Webbook
ripol	1323.00	NIST Webbook
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ripol	1284.00	NIST Webbook
ripol	1295.00	NIST Webbook
ripol	1295.00	NIST Webbook
ripol	1298.00	NIST Webbook
ripol	1272.00	NIST Webbook
ripol	1272.00	NIST Webbook
ripol	1272.00	NIST Webbook
ripol	1300.00	NIST Webbook
ripol	1295.00	NIST Webbook
ripol	1300.00	NIST Webbook
ripol	1268.00	NIST Webbook
ripol	1300.00	NIST Webbook
ripol	1323.00	NIST Webbook
ripol	1301.00	NIST Webbook
ripol	1308.00	NIST Webbook
ripol	1290.00	NIST Webbook
ripol	1296.00	NIST Webbook
ripol	1289.00	NIST Webbook
ripol	1315.00	NIST Webbook
ripol	1301.00	NIST Webbook

tb	418.70	K	NIST Webbook
tc	589.06	K	Joback Method
tf	234.32	K	Joback Method
vc	0.229	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.21	J/mol×K	589.06	Joback Method
cpg	116.00	J/mol×K	443.25	Joback Method
cpg	121.03	J/mol×K	472.41	Joback Method
cpg	125.86	J/mol×K	501.57	Joback Method
cpg	130.50	J/mol×K	530.74	Joback Method
cpg	134.95	J/mol×K	559.90	Joback Method
cpg	110.78	J/mol×K	414.09	Joback Method
dvisc	0.0005205	Pa×s	384.13	Joback Method
dvisc	0.0009143	Pa×s	354.17	Joback Method
dvisc	0.0017827	Pa×s	324.20	Joback Method
dvisc	0.0039819	Pa×s	294.24	Joback Method
dvisc	0.0106718	Pa×s	264.28	Joback Method
dvisc	0.0003214	Pa×s	414.09	Joback Method
dvisc	0.0368027	Pa×s	234.32	Joback Method
hvapt	42.00 ± 3.00	kJ/mol	326.00	NIST Webbook
pvap	0.17	kPa	278.55	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.36	kPa	289.86	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K

pvap	0.36	kPa	290.70	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.36	kPa	290.70	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.36	kPa	290.70	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.43	kPa	293.26	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.52	kPa	295.86	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.49	kPa	295.86	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.20	kPa	280.90	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K

pvap	0.62	kPa	300.30	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.64	kPa	301.20	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.72	kPa	302.11	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.75	kPa	303.03	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.82	kPa	303.95	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.21	kPa	281.69	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.20	kPa	281.69	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K

pvap	0.13	kPa	273.22	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.14	kPa	275.48	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.16	kPa	277.78	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.17	kPa	278.55	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
pvap	0.53	kPa	296.74	Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K
rfi	1.42620		293.15	Liquid-liquid equilibria of water + solutes (acetic acid/ acetol/furfural/guaiacol/methanol/phenol/propanal) + solvents (isopropyl acetate/toluene) ternary systems for pyrolysis oil fractionation
rhol	1047.55	kg/m3	323.15	Liquid-liquid equilibria and COSMO-SAC modeling of organic solvent/ ionic liquid - hydroxyacetone - water mixtures

rhol	1042.01	kg/m3	328.15	Liquid-liquid equilibria and COSMO-SAC modeling of organic solvent/ ionic liquid - hydroxyacetone - water mixtures	
rhol	1053.13	kg/m3	318.15	Liquid-liquid equilibria and COSMO-SAC modeling of organic solvent/ ionic liquid - hydroxyacetone - water mixtures	
rhol	1058.71	kg/m3	313.15	Liquid-liquid equilibria and COSMO-SAC modeling of organic solvent/ ionic liquid - hydroxyacetone - water mixtures	
rhol	1064.31	kg/m3	308.15	Liquid-liquid equilibria and COSMO-SAC modeling of organic solvent/ ionic liquid - hydroxyacetone - water mixtures	
rhol	1069.67	kg/m3	303.15	Liquid-liquid equilibria and COSMO-SAC modeling of organic solvent/ ionic liquid - hydroxyacetone - water mixtures	
rhol	1074.92	kg/m3	298.15	Liquid-liquid equilibria and COSMO-SAC modeling of organic solvent/ ionic liquid - hydroxyacetone - water mixtures	
rhol	1036.62	kg/m3	333.15	Liquid-liquid equilibria and COSMO-SAC modeling of organic solvent/ ionic liquid - hydroxyacetone - water mixtures	

rhol	1080.13	kg/m3	293.15	Liquid-liquid equilibria and COSMO-SAC modeling of organic solvent/ ionic liquid - hydroxyacetone - water mixtures

Sources

Vapor Pressure Measurements of Hydroxyacetaldehyde and Hydroxyacetone in the Temperature Range (273 to 356) K:	https://www.doi.org/10.1021/je9004905
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116096&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid-liquid equilibria and COSMO-SAC modeling of organic solvent/ ionic liquid - hydroxyacetone - water mixtures:	https://www.doi.org/10.1016/j.fluid.2018.01.026
Liquid-liquid equilibria of water + solutes (acetic acid/ acetol/furfural/guaiacol/methanol/phenol/propanal) + solvents (isopropyl acetate/toluene) ternary systems for pyrolysis oil fractionation:	https://www.doi.org/10.1016/j.fluid.2018.04.016

Legend

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
rfi:	Refractive Index
rhol:	Liquid Density
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