5-Hydroxymethylfurfural

Other names:	2-Furaldehyde, 5-(hydroxymethyl)-
	2-Furancarboxaldehyde, 5-(hydroxymethyl)-
	2-Hydroxymethyl-5-furfural
	5-(Hyddroxymethyl)furfurole
	5-(Hydroxymethyl)-2-formylfuran
	5-(Hydroxymethyl)-2-furancarbonal
	5-(Hydroxymethyl)-2-furancarboxaldehyde
	5-(Hydroxymethyl)-2-furfural
	5-(Hydroxymethyl)-2-furfuraldehyde
	5-(Hydroxymethyl)furan-2-aldehyde
	5-(hydroxymethyl)-2-furaldehyde
	5-(hydroxymethyl)furan-2-carbaldehyde
	5-Hydroxymethyl-2-furancarbaldehyde
	5-Hydroxymethyl-2-furfural (HMF)
	5-Hydroxymethylfuraldehyde
	5-Hydroxymethylfurfuraldehyde
	5-Oxymethylfurfurole
	HMF
	Hydroxymethylfurfural
	Hydroxymethylfurfuralaldehyde
	Hydroxymethylfurfuraldehyde
	NSC 40738
Inchi:	InChI=1S/C6H6O3/c7-3-5-1-2-6(4-8)9-5/h1-3,8H,4H2
InchiKey:	NOEGNKMFWQHSLB-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	O=Cc1ccc(CO)o1
Mol. weight [g/mol]:	126.11
CAS:	67-47-0

Physical Properties

Property code	Value	Unit	Source
hvap	83.40 ± 0.20	kJ/mol	NIST Webbook
log10ws	-5.59		Crippen Method
logp	0.584		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
rinpol	1238.00		NIST Webbook

rinpol	1200.00	NIST Webbook
rinpol	1218.00	NIST Webbook
rinpol	1233.20	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1188.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1266.00	NIST Webbook
rinpol	1235.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1224.00	NIST Webbook
rinpol	1231.00	NIST Webbook
rinpol	1225.00	NIST Webbook
rinpol	1228.00	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1196.00	NIST Webbook
rinpol	1195.00	NIST Webbook
rinpol	1200.00	NIST Webbook
rinpol	1200.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1241.00	NIST Webbook
rinpol	1226.00	NIST Webbook
rinpol	1238.00	NIST Webbook
rinpol	1230.00	NIST Webbook
rinpol	1230.00	NIST Webbook
rinpol	1230.00	NIST Webbook
rinpol	1234.00	NIST Webbook
rinpol	1218.00	NIST Webbook
rinpol	1200.00	NIST Webbook
rinpol	1233.20	NIST Webbook
rinpol	1208.00	NIST Webbook
rinpol	1224.00	NIST Webbook
rinpol	1236.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1225.00	NIST Webbook
rinpol	1236.00	NIST Webbook
rinpol	1266.00	NIST Webbook
ripol	2515.00	NIST Webbook
ripol	2485.00	NIST Webbook
ripol	2532.00	NIST Webbook
ripol	2496.00	NIST Webbook
ripol	2495.00	NIST Webbook
ripol	2509.00	NIST Webbook

ripol	2505.00	NIST Webbook
ripol	2530.00	NIST Webbook
ripol	2501.00	NIST Webbook
ripol	2511.00	NIST Webbook
ripol	2515.00	NIST Webbook
ripol	2528.00	NIST Webbook
ripol	2466.00	NIST Webbook
ripol	2509.00	NIST Webbook
ripol	2515.00	NIST Webbook
ripol	2485.00	NIST Webbook
ripol	2490.00	NIST Webbook
ripol	2505.00	NIST Webbook
ripol	2512.00	NIST Webbook
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ripol	2469.00	NIST Webbook
ripol	2482.00	NIST Webbook
ripol	2530.00	NIST Webbook
ripol	2474.00	NIST Webbook
ripol	2487.00	NIST Webbook
ripol	2537.00	NIST Webbook
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ripol	2494.00	NIST Webbook
ripol	2493.00	NIST Webbook
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ripol	2492.00	NIST Webbook
ripol	2509.00	NIST Webbook
ripol	2532.00	NIST Webbook
ripol	2485.00	NIST Webbook
ripol	2513.00	NIST Webbook
ripol	2496.00	NIST Webbook
ripol	2526.00	NIST Webbook
ripol	2496.00	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	19.80	kJ/mol	308.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.20	K	0.10	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Osmotic coefficients and activity coefficients in binary water/5-(hydroxymethyl)furfural and in ternary water/5-(hydroxymethyl)furfural/salt solutions at 298.15 K:	https://www.doi.org/10.1016/j.jct.2019.105878
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermophysical Properties and Solubility of Different Sugar-Derived Molecules in Deep Eutectic Solvents:	https://www.doi.org/10.1021/acs.jced.7b00184
Liquid-liquid equilibrium for (water + 5-hydroxymethylfurfural + 1-pentanol or 1-hexanol or 1-heptanol) systems at 298.15 K:	https://www.doi.org/10.1016/j.jct.2019.06.010
Influence of electrolytes on liquid-liquid equilibria of water/1-butanol and on the partitioning of 5-hydroxymethylfurfural in water/1-butanol:	https://www.doi.org/10.1016/j.fluid.2016.05.001
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Liquid-liquid equilibrium in systems used for the production of 5-hydroxymethylfurfural from biomass using alcohols as solvents:	https://www.doi.org/10.1016/j.jct.2017.03.019
Solubility of 5-Hydroxymethylfurfural in Supercritical Carbon Dioxide with and without Ethanol as Cosolvent at (314.1 to 343.2) K:	https://www.doi.org/10.1021/je100985n
Thermodynamic properties of hydrophobic deep eutectic solvents and solubility of water and HMF in them: Measurements and COSMO-SAC modeling:	https://www.doi.org/10.1016/j.fluid.2019.02.010
Salt effect on liquid-liquid equilibria of tetrahydrofuran/water/5-hydroxymethylfurfural at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2019.04.018
Biomass-Derived Platform Chemicals:	https://www.doi.org/10.1021/je300529j
Thermodynamic Studies on the Extraction of 5-Hydroxymethylfurfural (HMF) from Ionic Liquids:	https://www.doi.org/10.1016/j.fluid.2018.07.034
Liquid-liquid equilibria of ternary and quaternary systems involving 5-hydroxymethylfurfural, water, organic solvents, and salts at 313.15 K and atmospheric pressure:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67470&Units=SI
NIST Webbook:	
Infinite Dilution Binary Diffusion Coefficients for Compounds Derived from Biomass in Water at 0.1 MPa and Temperatures from (298.2 to 353.2) K:	https://www.doi.org/10.1021/je301060a
Liquid-Liquid Equilibrium for Ternary Systems Water + 5-Hydroxymethylfurfural + (1-Butanol, Isobutanol, Methyl Isobutyl Ketone), at 313.15, 323.15, and 333.15 K:	https://www.doi.org/10.1021/acs.jced.8b00120

Legend

hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tbrp:	Boiling point at reduced pressure