Pentanoic acid, 4-oxo-

Other names:	.beta.-acetylpropionic acid
	3-Acetylpropionic acid
	4-Ketovaleric acid
	4-Oxo-pentanoic acid (levulinic acid)
	4-Oxovaleric acid
	4-oxopentanoic acid
	Acetopropionic acid
	Acetylpropionic acid
	LEVA
	Laevulic acid
	Laevulinic acid
	Levulic acid
	NSC 3716
	Propionic acid, 3-acetyl-
	USAF CZ-1
	Valeric acid, 4-oxo-
	Valeric acid, 4-oxo-(levulinic acid)
	levulinic acid
	«beta»-Acetylpropionic acid
	«gamma»-Ketovaleric acid
Inchi:	InChI=1S/C5H8O3/c1-4(6)2-3-5(7)8/h2-3H2,1H3,(H,7,8)
InchiKey:	JOOXCMJARBKPKM-UHFFFAOYSA-N
Formula:	C5H8O3
SMILES:	CC(=O)CCC(=O)O
Mol. weight [g/mol]:	116.12
CAS:	123-76-2

Physical Properties

Property code	Value	Unit	Source
gf	-403.44	kJ/mol	Joback Method
hf	-523.92	kJ/mol	Joback Method
hfus	15.99	kJ/mol	Joback Method
hvap	56.89	kJ/mol	Joback Method
log10ws	-0.29		Crippen Method
logp	0.440		Crippen Method
mcvol	90.320	ml/mol	McGowan Method
pc	4565.38	kPa	Joback Method

rinpol	1063.20		NIST Webbook
rinpol	1063.20		NIST Webbook
ripol	2312.00		NIST Webbook
ripol	2340.00		NIST Webbook
ripol	2317.00		NIST Webbook
ripol	2317.00		NIST Webbook
tb	518.20	K	Phase equilibria of (water + levunilic acid + alcohol) ternary systems
tb	518.70	K	NIST Webbook
tc	695.98	K	Joback Method
tf	306.00 ± 2.00	K	NIST Webbook
tf	310.00 ± 1.00	K	NIST Webbook
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.80	J/mol×K	513.72	Joback Method
cpg	201.95	J/mol×K	544.10	Joback Method
cpg	208.77	J/mol×K	574.47	Joback Method
cpg	215.27	J/mol×K	604.85	Joback Method
cpg	221.47	J/mol×K	635.23	Joback Method
cpg	227.36	J/mol×K	665.60	Joback Method
cpg	232.95	J/mol×K	695.98	Joback Method
dvisc	0.0002045	Pa×s	513.72	Joback Method
dvisc	0.0038842	Pa×s	341.28	Joback Method
dvisc	0.0017366	Pa×s	375.77	Joback Method
dvisc	0.0104113	Pa×s	306.79	Joback Method
dvisc	0.0005049	Pa×s	444.74	Joback Method
dvisc	0.0003110	Pa×s	479.23	Joback Method
dvisc	0.0008890	Pa×s	410.25	Joback Method
hfust	9.22	kJ/mol	306.20	NIST Webbook
hfust	9.22	kJ/mol	306.20	NIST Webbook
hvapt	70.32	kJ/mol	298.15	Renewable platform-chemicals and materials: Thermochemical study of levulinic acid
hvapt	74.40	kJ/mol	447.00	NIST Webbook

rfi	1.43950		293.15	Phase equilibria of (water + levulinic acid + dibasic esters) ternary systems
rhol	1135.71	kg/m3	298.15	Extraction of Carboxylic Acids from Aqueous Solutions by Using [BMim][NTf2] and Salting-out Agents

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid-liquid equilibria for ternary systems of (water + carboxylic acid + 1-octanol) at 293.15 K: modeling phase equilibria using a solvatochromic approach:	https://www.doi.org/10.1016/j.fluid.2004.10.029
Investigation of solubilities of carbon dioxide in five levulinic acid-based cyclic solvents at T = 298.2 K:	https://www.doi.org/10.1016/j.jct.2016.08.015
Phase equilibria for ternary liquid systems (water + levulinic acid + cyclic solvent) at T = 298.2 K:	https://www.doi.org/10.1016/j.jct.2005.01.014
Thermodynamic properties:	https://www.doi.org/10.1016/j.fluid.2009.04.017
Phase equilibria of (water + levulinic acid + dibasic esters) ternary systems:	https://www.doi.org/10.1021/acs.jced.8b00335
Liquid-Liquid Equilibria of Formic Acid and Furfural in a Biphasic Aqueous-Organic System: Optimization of Solvent and Amine Extractant:	https://www.doi.org/10.1016/j.fluid.2018.08.020
Thermodynamic model:	https://en.wikipedia.org/wiki/Joback_method
liquid-liquid equilibria of n-heptane, methanol, and deep eutectic solvents composed of carboxylic acid and monocyclic terpenes:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://www.doi.org/10.1016/j.fluid.2008.08.004
McGowan Method:	https://www.doi.org/10.1016/j.jct.2018.12.017
Phase equilibria of (water + levulinic acid + alcohol) ternary systems:	https://www.doi.org/10.1021/acs.jced.6b00164
Physical properties of seven deep eutectic solvents based on L-proline or betaine:	https://www.doi.org/10.1021/je900727r
Equilibrium Study on the Extraction of Levulinic Acid from Aqueous Solution with Aliquat 336 Dissolved in Different Solvents and Its Ternary Liquid Equilibrium Data:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123762&Units=SI
Levulinic Acid Solubility in Supercritical Carbon Dioxide with and without Ethanol as Cosolvent at Different Temperatures:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	https://www.doi.org/10.1016/j.tca.2017.12.006
Column Design:	https://www.doi.org/10.1021/acs.jced.7b00184
Crippen Method:	https://www.doi.org/10.1021/acs.jced.8b01023
Renewable platform chemicals: Thermochemical study of levulinic acid esters:	https://www.doi.org/10.1021/acs.jced.9b00041
Thermophysical Properties and Solubility of Different Sugar-Derived Molecules in Deep Eutectic Solvents:	https://www.doi.org/10.1021/acs.jced.6b00563
Phase Equilibrium Measurements and Thermodynamic Modeling of the Systems (CO2 + Ethyl Levulinate) and (CO2 + Levulinic Acid):	https://www.doi.org/10.1021/je400814n
Extraction of Carboxylic Acids from Aqueous Solutions by Using [BMim][NTf2] and Salting-out Agents:	https://www.doi.org/10.1016/j.jct.2011.07.014
Physical Properties of the Pure Deep Eutectic Solvent, [ChCl]:[Lev] (1:2) DES, and Its Binary Mixtures with Alcohols:	https://www.doi.org/10.1016/j.jct.2017.12.008
Phase Equilibria in Systems with Levulinic Acid and Ethyl Levulinate:	
Renewable platform-chemicals and materials: Thermochemical study of levulinic acid:	
Liquid-liquidequilibria for the aqueous mixture of C5 carboxylic acids and heavier than water solvents at T = 298.2 K:	

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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