Pentanoic acid, 4-oxo-, ethyl ester

Other names:	4-Oxopentanoic acid ethyl ester
	Ethyl 3-acetylpropionate
	Ethyl 4-ketovalerate
	Ethyl 4-oxopentanoate
	Ethyl 4-oxovalerate
	Ethyl ketovalerate
	Ethyl laevulinate
	Ethyl levulate
	Ethyl levulinate
	Levulinic acid, ethyl ester
	NSC 24876
Inchi:	InChI=1S/C7H12O3/c1-3-10-7(9)5-4-6(2)8/h3-5H2,1-2H3
InchiKey:	GMEONFUTDYJSNV-UHFFFAOYSA-N
Formula:	C7H12O3
SMILES:	CCOC(=O)CCC(C)=O
Mol. weight [g/mol]:	144.17
CAS:	539-88-8

Physical Properties

Property code	Value	Unit	Source
gf	-354.78	kJ/mol	Joback Method
hf	-545.19	kJ/mol	Joback Method
hfus	18.27	kJ/mol	Joback Method
hvap	47.08	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.919		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
rinpol	1023.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1029.00		NIST Webbook
ripol	1607.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1567.00		NIST Webbook

ripol	1601.00		NIST Webbook
ripol	1607.00		NIST Webbook
ripol	1614.00		NIST Webbook
ripol	1607.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1607.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1607.00		NIST Webbook
tb	479.00	K	NIST Webbook
tc	676.50	K	Joback Method
tf	290.74	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.79	J/mol×K	489.72	Joback Method
cpg	266.32	J/mol×K	520.85	Joback Method
cpg	276.45	J/mol×K	551.98	Joback Method
cpg	286.16	J/mol×K	583.11	Joback Method
cpg	295.47	J/mol×K	614.24	Joback Method
cpg	304.37	J/mol×K	645.37	Joback Method
cpg	312.87	J/mol×K	676.50	Joback Method
dvisc	0.0027292	Pa×s	290.74	Joback Method
dvisc	0.0015623	Pa×s	323.90	Joback Method
dvisc	0.0009920	Pa×s	357.07	Joback Method
dvisc	0.0006804	Pa×s	390.23	Joback Method
dvisc	0.0004951	Pa×s	423.39	Joback Method
dvisc	0.0003773	Pa×s	456.56	Joback Method
dvisc	0.0002983	Pa×s	489.72	Joback Method
hvapt	51.60	kJ/mol	420.00	NIST Webbook
hvapt	58.30	kJ/mol	400.00	NIST Webbook
pvap	0.08	kPa	313.30	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.02	kPa	293.50	Renewable platform chemicals: Thermochemical study of levulinic acid esters

pvap	0.03	kPa	298.40	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.04	kPa	303.30	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.05	kPa	308.30	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.76	kPa	348.80	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.55	kPa	343.10	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.41	kPa	338.10	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.31	kPa	333.10	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.23	kPa	328.20	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.16	kPa	323.30	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.11	kPa	318.30	Renewable platform chemicals: Thermochemical study of levulinic acid esters

rhol	1005.30	kg/m3	303.15	Solubilities and thermodynamic properties of SO2 in five biobased solvents
rhol	1007.54	kg/m3	298.15	Self-aggregation of liquids from biomass in aqueous solution
rhol	975.10	kg/m3	333.15	Solubilities and thermodynamic properties of SO2 in five biobased solvents
rhol	984.60	kg/m3	323.15	Solubilities and thermodynamic properties of SO2 in five biobased solvents
rhol	1013.20	kg/m3	293.15	Solubilities and thermodynamic properties of SO2 in five biobased solvents
rhol	994.90	kg/m3	313.15	Solubilities and thermodynamic properties of SO2 in five biobased solvents

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	366.70	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51235e+01
Coeff. B	-4.24496e+03
Coeff. C	-7.48680e+01
Temperature range (K), min.	361.00
Temperature range (K), max.	507.50

Sources

Self-aggregation of liquids from biomass in aqueous solution:	https://www.doi.org/10.1016/j.jct.2013.06.020
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Renewable platform chemicals:	https://www.doi.org/10.1016/j.tca.2017.12.006
Thermochemical study of levulinic acid esters:	https://www.doi.org/10.1021/je400814n
Phase Equilibria in Systems with Levulinic Acid and Ethyl Levulinate:	https://www.doi.org/10.1021/je500812s
Solubilities of Carbon Dioxide in Five Bio-based Solvents:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
The Yaws Handbook of Vapor Pressure:	https://www.doi.org/10.1016/j.jct.2015.09.017
Solubilities and thermodynamic properties of SO2 in five biobased solvents:	http://link.springer.com/article/10.1007/BF02311772
McGowan Method:	https://www.doi.org/10.1021/acs.jced.8b01023
Phase Equilibrium Measurements and Thermodynamic Modeling of the Systems (CO2 + Ethyl Levulinate) and (CO2 + Levulinic Acid):	https://en.wikipedia.org/wiki/Joback_method
Joback Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C539888&Units=SI
NIST Webbook:	

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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