2-Propenoic acid

Other names:	ACROLEIC ACID
	ACRYLIC ACID
	CH2=CHCOOH
	ETHYLENECARBOXYLIC ACID
	Glacial acrylic acid
	Kyselina akrylova
	NSC 4765
	PROPENOIC ACID
	Propene acid
	Rcra waste number U008
	Vinylformic acid
Inchi:	InChI=1S/C3H4O2/c1-2-3(4)5/h2H,1H2,(H,4,5)
InchiKey:	NIXOWILDQLNWCW-UHFFFAOYSA-N
Formula:	C3H4O2
SMILES:	C=CC(=O)O
Mol. weight [g/mol]:	72.06
CAS:	79-10-7

Physical Properties

Property code	Value	Unit	Source
af	0.5600		KDB
aigt	463.15	K	KDB
chl	-1373.00 ± 5.00	kJ/mol	NIST Webbook
chl	-1368.80 ± 1.80	kJ/mol	NIST Webbook
chl	-1374.00 ± 11.00	kJ/mol	NIST Webbook
fll	2.40	% in Air	KDB
fpc	320.93	K	KDB
gf	-286.30	kJ/mol	KDB
hf	-330.70 ± 4.20	kJ/mol	NIST Webbook
hf	-336.90 ± 2.30	kJ/mol	NIST Webbook
hf	-324.70	kJ/mol	NIST Webbook
hf	-336.50	kJ/mol	KDB
hfl	-377.80 ± 9.30	kJ/mol	NIST Webbook
hfl	-383.80 ± 2.00	kJ/mol	NIST Webbook
hfus	7.93	kJ/mol	Joback Method
hvap	53.10 ± 4.20	kJ/mol	NIST Webbook
hvap	53.10	kJ/mol	NIST Webbook

hvap	53.10 ± 4.20	kJ/mol	NIST Webbook
hvap	57.30	kJ/mol	NIST Webbook
hvap	57.30 ± 1.30	kJ/mol	NIST Webbook
ie	10.78	eV	NIST Webbook
ie	10.60	eV	NIST Webbook
ie	10.60	eV	NIST Webbook
ie	10.60	eV	NIST Webbook
log10ws	-0.03		Crippen Method
logp	0.257		Crippen Method
mcvol	56.270	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=3)		KDB
nfpas	%!d(float64=2)		KDB
pc	5242.73 ± 100.00	kPa	NIST Webbook
pc	5670.00	kPa	KDB
tb	414.80	K	NIST Webbook
tb	414.45	K	NIST Webbook
tb	414.00	K	KDB
tb	412.20	K	NIST Webbook
tc	616.57 ± 3.00	K	NIST Webbook
tc	615.00	K	KDB
tf	285.45 ± 0.50	K	NIST Webbook
tf	285.00	K	KDB
tf	285.70 ± 0.20	K	NIST Webbook
tf	285.45	K	NIST Webbook
tf	285.30 ± 0.60	K	NIST Webbook
tf	290.00 ± 1.00	K	NIST Webbook
tf	285.70	K	NIST Webbook
vc	0.210	m3/kmol	KDB
zc	0.2328580		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	100.76	J/mol×K	440.54	Joback Method
cpg	105.01	J/mol×K	470.31	Joback Method
cpg	96.30	J/mol×K	410.77	Joback Method
cpg	120.07	J/mol×K	589.38	Joback Method
cpg	116.59	J/mol×K	559.61	Joback Method
cpg	112.92	J/mol×K	529.84	Joback Method
cpg	109.06	J/mol×K	500.08	Joback Method

cpl	145.70	J/mol×K	300.00	NIST Webbook
cpl	144.20	J/mol×K	298.15	NIST Webbook
dvisc	0.0100054	Pa×s	262.26	Joback Method
dvisc	0.0038034	Pa×s	291.96	Joback Method
dvisc	0.0017285	Pa×s	321.66	Joback Method
dvisc	0.0008976	Pa×s	351.37	Joback Method
dvisc	0.0005163	Pa×s	381.07	Joback Method
dvisc	0.0003216	Pa×s	410.77	Joback Method
dvisc	0.0336978	Pa×s	232.56	Joback Method
hfust	9.51	kJ/mol	285.70	NIST Webbook
hfust	11.16	kJ/mol	285.50	NIST Webbook
hfust	11.16	kJ/mol	285.50	NIST Webbook
hvapt	45.30	kJ/mol	377.50	NIST Webbook
hvapt	46.02	kJ/mol	414.00	KDB
hvapt	32.70	kJ/mol	318.00	NIST Webbook
pvap	20.00	kPa	368.40	Isobaric Vapor Liquid Equilibrium for Binary Systems of Toluene + Acrylic Acid, Toluene + Acetic Acid, and Cyclohexane + Acrylic Acid at 20 kPa
rhol	1059.17	kg/m3	298.15	Evaluation of the Performance of Four Solvents for the Liquid Liquid Extraction of Acrylic Acid from Water
rhol	1051.00	kg/m3	293.00	KDB
rhol	1051.22	kg/m3	293.15	Measurements and Comparative Study of Ternary Liquid Liquid Equilibria for Water + Acrylic Acid + Cyclopentyl Methyl Ether at (293.15, 303.15, and 313.15) K and 100.249 kPa
sfust	33.30	J/mol×K	285.70	NIST Webbook

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62275e+01
Coeff. B	-4.24500e+03
Coeff. C	-4.65410e+01
Temperature range (K), min.	286.65
Temperature range (K), max.	437.98

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.61842e+01
Coeff. B	-7.35729e+03
Coeff. C	-5.66895e+00
Coeff. D	2.19318e-06
Temperature range (K), min.	286.65
Temperature range (K), max.	615.00

Sources

Measurement and modelling of urea solubility in aqueous	https://www.doi.org/10.1016/j.jct.2016.08.009
Measurements and Comparative Study of Ternary Liquid Liquid Equilibria for Water + Acrylic Acid + Cyclopentyl Methyl Ether at (293.15, 303.15, and 313.15) K and 100/249 kPa:	https://www.doi.org/10.1021/je501085y
Propane-1,2,3-triol and prop-2-enoic acid solutions:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
The Yaws Handbook of Vapor Pressure:	https://www.doi.org/10.1021/acs.jced.5b00500
Isobaric Vapor-Liquid-Liquid Equilibrium for Water + Cyclohexane + Acrylic Acid at 200 mmHg:	https://www.doi.org/10.1021/je2003226
Ternary Liquid-Liquid Equilibria of Water + Prop-2-enoic Acid + Isobutyl Ethanoate at Different Temperatures :	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=972
KDB:	https://www.doi.org/10.1021/je201130h
Evaluation of the Performance of Four Solvents for the Liquid Liquid Extraction of Acrylic Acid from Water:	https://www.doi.org/10.1021/je200655s
Isobaric Vapor-Liquid Equilibrium for Binary Systems of Toluene + Acrylic Acid, Toluene + Acetic Acid, and Cyclohexane + Acrylic Acid at 20 kPa:	https://www.doi.org/10.1016/j.fluid.2018.07.024
Solubility determination and correlation of cytarabine in sixteen pure solvents and mixing properties of solutions:	https://en.wikipedia.org/wiki/Joback_method
Joback Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79107&Units=SI
NIST Webbook:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=972
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=972
KDB Vapor Pressure Data:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	https://www.doi.org/10.1021/je700439n
Liquid Liquid Equilibria of the Ternary System Water + Acrylic Acid + 4-Methyl-2-pentanone at 298.15 K:	http://link.springer.com/article/10.1007/BF02311772
McGowan Method:	https://www.doi.org/10.1016/j.jct.2011.04.009
(Liquid + liquid) equilibria in {water + acrylic acid + (1-butanol, or 2-butanol, or 1-pentanol)} systems at T = 293.2 K, T = 303.2 K, and T = 313.2 K and atmospheric pressure:	

Legend

af:	Acentric Factor
aigt:	Autoignition Temperature
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
fll:	Lower Flammability Limit
fpc:	Flash Point (Closed Cup Method)
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility