Propargyl alcohol

Other names:	1-Hydroxy-2-propyne
	1-Propyn-3-ol
	1-Propyn-3-yl alcohol
	1-Propyne-3-ol
	2-Propyn-1-ol
	2-Propynol
	2-Propynyl alcohol
	2-propyn-1-ol (propargyl alcohol)
	3-Hydroxy-1-propyne
	3-Propynol
	Ethynyl carbinol
	HC«equiv»CCH2OH
	HCÂ«equivÂ»CCH2OH
	Methanol, ethynyl-
	NSC 8804
	Propynyl alcohol
	Rcra waste number P102
	prop-2-yn-1-ol
Inchi:	InChI=1S/C3H4O/c1-2-3-4/h1,4H,3H2
InchiKey:	TVDSBUOJIPERQY-UHFFFAOYSA-N
Formula:	C3H4O
SMILES:	C#CCO
Mol. weight [g/mol]:	56.06
CAS:	107-19-7

Physical Properties

Property code	Value	Unit	Source
gf	60.63	kJ/mol	Joback Method
hf	34.42	kJ/mol	Joback Method
hfus	10.59	kJ/mol	Joback Method
hvap	38.81	kJ/mol	Joback Method
ie	10.51	eV	NIST Webbook
ie	10.50	eV	NIST Webbook
ie	10.45	eV	NIST Webbook
ie	10.50	eV	NIST Webbook
log10ws	-0.14		Crippen Method
logp	-0.388		Crippen Method

mcvol	50.400	ml/mol	McGowan Method
pc	6239.25	kPa	Joback Method
rinpol	559.00		NIST Webbook
rinpol	552.00		NIST Webbook
rinpol	569.00		NIST Webbook
rinpol	546.00		NIST Webbook
rinpol	576.00		NIST Webbook
rinpol	566.00		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	552.00		NIST Webbook
rinpol	576.00		NIST Webbook
rinpol	546.00		NIST Webbook
ripol	1357.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1352.00		NIST Webbook
ripol	1343.00		NIST Webbook
ripol	1352.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1343.00		NIST Webbook
ripol	1334.00		NIST Webbook
tb	385.00 ± 3.00	K	NIST Webbook
tb	386.75 ± 0.50	K	NIST Webbook
tb	386.80	K	NIST Webbook
tb	387.50 ± 0.50	K	NIST Webbook
tc	523.88	K	Joback Method
tf	221.35 ± 0.30	K	NIST Webbook
vc	0.184	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	81.35	J/mol×K	350.34	Joback Method
cpg	85.08	J/mol×K	379.26	Joback Method
cpg	88.64	J/mol×K	408.19	Joback Method
cpg	92.02	J/mol×K	437.11	Joback Method
cpg	95.25	J/mol×K	466.04	Joback Method
cpg	98.32	J/mol×K	494.96	Joback Method
cpg	101.24	J/mol×K	523.88	Joback Method
hvapt	42.00	kJ/mol	340.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.46079e+01
Coeff. B	-7.44693e+03
Coeff. C	-8.68936e+00
Coeff. D	6.86908e-06
Temperature range (K), min.	221.35
Temperature range (K), max.	580.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Liquid-liquid equilibrium study for ternary systems of water + propargyl alcohol + solvents at 308.2 K:	https://www.doi.org/10.1016/j.jct.2019.03.033
Determination of Henry's Law Constants Using Internal Standards with Measured and Thermodynamic Values:	https://www.doi.org/10.1021/je3010535
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid-liquid equilibrium of the ternary system water p propargyl alcohol p n propyl acetate:	https://www.doi.org/10.1016/j.fluid.2016.10.023
Modelling:	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol894.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107197&Units=SI
Liquid liquid equilibrium of ternary mixture (propargyl alcohol +water + butyl acetate):	https://www.doi.org/10.1016/j.fluid.2009.04.010
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=894
Liquid liquid equilibria of ternary mixture (propargyl alcohol + diisopropyl ether +water):	https://www.doi.org/10.1016/j.fluid.2007.07.015
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
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