1-Pentyne

Other names:	Acetylene, propyl-
	C3H7C«equiv»CH
	C3H7CÂ«equivÂ»CH
	PROPYLACETYLENE
	pent-1-yne
Inchi:	InChI=1S/C5H8/c1-3-5-4-2/h1H,4-5H2,2H3
InchiKey:	IBXNCJKFFQIKKY-UHFFFAOYSA-N
Formula:	C5H8
SMILES:	C#CCCC
Mol. weight [g/mol]:	68.12
CAS:	627-19-0

Physical Properties

Property code	Value	Unit	Source
af	0.1640		KDB
dm	0.90	debye	KDB
gf	210.40	kJ/mol	KDB
hcg	3226.62	kJ/mol	KDB
hcn	3050.554	kJ/mol	KDB
hf	144.40	kJ/mol	KDB
hf	144.30 ± 2.10	kJ/mol	NIST Webbook
hfus	11.68	kJ/mol	Joback Method
hvap	28.40	kJ/mol	NIST Webbook
ie	10.10 ± 0.01	eV	NIST Webbook
ie	10.10 ± 0.02	eV	NIST Webbook
ie	10.10 ± 0.01	eV	NIST Webbook
ie	10.05	eV	NIST Webbook
log10ws	-1.64		Estimated Solubility Method
log10ws	-1.64		Aqueous Solubility Prediction Method
logp	1.420		Crippen Method
mcvol	72.710	ml/mol	McGowan Method
pc	4050.00	kPa	KDB
rinpol	484.00		NIST Webbook
rinpol	509.00		NIST Webbook
rinpol	484.00		NIST Webbook

rinpol	484.00		NIST Webbook
rinpol	484.40		NIST Webbook
rinpol	484.50		NIST Webbook
rinpol	484.00		NIST Webbook
rinpol	484.40		NIST Webbook
rinpol	484.80		NIST Webbook
rinpol	484.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	510.00		NIST Webbook
rinpol	484.50		NIST Webbook
rinpol	484.00		NIST Webbook
rinpol	509.00		NIST Webbook
rinpol	484.00		NIST Webbook
rinpol	484.00		NIST Webbook
tb	313.15 ± 1.00	K	NIST Webbook
tb	313.15 ± 1.50	K	NIST Webbook
tb	312.95 ± 1.00	K	NIST Webbook
tb	312.90 ± 0.80	K	NIST Webbook
tb	313.15 ± 0.70	K	NIST Webbook
tb	312.15 ± 1.00	K	NIST Webbook
tb	312.85 ± 0.60	K	NIST Webbook
tb	313.33	K	KDB
tb	313.00	K	NIST Webbook
tb	313.40	K	NIST Webbook
tb	312.80 ± 2.00	K	NIST Webbook
tb	313.38 ± 0.20	K	NIST Webbook
tb	313.33 ± 0.20	K	NIST Webbook
tb	312.20 ± 1.00	K	NIST Webbook
tb	312.85 ± 1.00	K	NIST Webbook
tb	312.65 ± 2.00	K	NIST Webbook
tb	313.35 ± 0.40	K	NIST Webbook
tb	313.40 ± 0.20	K	NIST Webbook
tb	315.15 ± 2.00	K	NIST Webbook
tb	313.35 ± 0.30	K	NIST Webbook
tb	312.65 ± 1.50	K	NIST Webbook
tb	312.45 ± 0.50	K	NIST Webbook
tb	313.15 ± 1.00	K	NIST Webbook
tc	493.50	K	KDB
tf	167.08 ± 0.20	K	NIST Webbook
tf	183.00	K	KDB
tf	172.48	K	Aqueous Solubility Prediction Method
tf	166.65 ± 0.30	K	NIST Webbook
vc	0.278	m3/kmol	KDB
zc	0.2743950		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.70	J/mol×K	420.17	Joback Method
cpg	141.82	J/mol×K	449.24	Joback Method
cpg	108.43	J/mol×K	303.92	Joback Method
cpg	115.69	J/mol×K	332.98	Joback Method
cpg	122.65	J/mol×K	362.05	Joback Method
cpg	129.31	J/mol×K	391.11	Joback Method
cpg	147.68	J/mol×K	478.30	Joback Method
hvapt	27.74	kJ/mol	313.40	KDB
hvapt	31.80	kJ/mol	272.00	NIST Webbook
rfi	1.38260		298.15	KDB
rhol	690.00	kg/m3	293.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39994e+01
Coeff. B	-2.38534e+03
Coeff. C	-5.90590e+01
Temperature range (K), min.	233.02
Temperature range (K), max.	333.62

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.86812e+01
Coeff. B	-5.16272e+03
Coeff. C	-6.64398e+00
Coeff. D	6.01492e-06
Temperature range (K), min.	167.45
Temperature range (K), max.	481.20

Sources

Activity Coefficients at Infinite Dilution Measurements for Organic Solutes and Water in the Ionic Liquid 1-Hexyl-3-methylimidazolium Thiocyanate	https://www.doi.org/10.1021/je900890u
The study of activity coefficients at infinite dilution for organic solutes and water in 1-butyl-4-methylpyridinium dicyanamide, [B4MPy][DCA] using GLC	https://www.doi.org/10.1016/j.jct.2013.09.007
Separation of binary mixtures hexane/hex-1-ene, cyclohexane/cyclohexene and ethylbenzene/styrene based on limiting activity coefficients	https://www.doi.org/10.1016/j.jct.2017.03.004
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Experimental and theoretical study on infinite dilution activity coefficients of various solutes in piperidinium ionic liquids	https://www.doi.org/10.1016/j.jct.2013.01.005
Thermodynamics and activity coefficients at infinite dilution for organic solutes and water in the ionic liquid 1-butyl-1-methylmorpholinium tricyanomethanide:	https://www.doi.org/10.1016/j.jct.2013.08.030
New ionic liquid [P4,4,4,4][NTf2] in bio-butanol extraction on investigation of limiting activity coefficients:	https://www.doi.org/10.1016/j.fluid.2018.07.028
Activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-butyl-3-methylimidazolium hexafluoroantimonate using gas-liquid chromatography at T = (313.15, 323.15, and 333.15) K	https://www.doi.org/10.1016/j.jct.2010.12.019
Activity coefficients at infinite dilution measurements for organic solutes in the ionic liquid 1-butyl-4-methylpyridinium tosylate using GLC at T = (328.15, 333.15, 338.15, and 348.15) K	https://www.doi.org/10.1016/j.fluid.2008.10.008
Activity coefficients at infinite dilution of organic solutes in the ionic liquid trihexyl(tetradecyl)phosphonium tetrafluoroborate using gas-liquid chromatography at T = (313.15, 333.15, 353.15 and 373.15) K	https://www.doi.org/10.1016/j.jct.2010.12.005
Activity coefficients at infinite dilution measurements for organic solutes and water in the ionic liquid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1016/j.jct.2008.12.005
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Thermodynamic study of molecular interaction-selectivity in separation processes based on limiting activity coefficients:	https://www.doi.org/10.1016/j.jct.2018.02.014
Activity coefficients at infinite dilution of organic solutes in N-formylmorpholine and N-methylpyrrolidone from gas-liquid chromatography:	https://www.doi.org/10.1016/j.jct.2013.02.006
Activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-hexyl-3-methylimidazolium hexafluorophosphate using gas-liquid chromatography at T = (313.15, 323.15, and 333.15) K	https://www.doi.org/10.1016/j.jct.2009.12.004
Measurement of activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-ethyl-3-methylimidazolium 2-(2-methoxyethoxy) ethylsulfate at T = (308.15, 313.15, 323.15 and 333.15) K using gas + liquid chromatography:	https://www.doi.org/10.1016/j.jct.2013.10.017
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Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=404
Measurements of activity coefficients at infinite dilution of aliphatic and aromatic hydrocarbons, alcohols, thiophene, tetrahydrofuran, MTBE, and water in ionic liquid [BMIM][SCN] using GLC:	https://www.doi.org/10.1016/j.jct.2008.12.018
Gas-liquid chromatography measurements of activity coefficients at infinite dilution of hydrocarbons and alkanols in 1-alkyl-3-methylimidazolium bis(oxalato)borate:	https://www.doi.org/10.1016/j.fluid.2010.08.016
Activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-ethyl-3-methylimidazolium trifluoromethanesulfonate using gas liquid chromatography at T = (313.15, 323.15, and 333.15) K	https://www.doi.org/10.1016/j.jct.2009.07.010
Activity coefficients at infinite dilution and physicochemical properties for organic solvents and water in the ionic liquid 4-(3-hydroxypropyl)-4-methylmorpholinium bis(trifluoromethylsulfonyl)-amide:	https://www.doi.org/10.1016/j.jct.2015.02.024
Activity coefficients at infinite dilution for organic solutes and water in 2-hydroxyethylammonium lactate:	https://www.doi.org/10.1016/j.jct.2015.05.014
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Determination of Activity Coefficients at Infinite Dilution of Organic Solutes in the Ionic Liquid 1-(2-Hydroxyethyl)-3-methylimidazolium Nonafluoro-1-butanesulfonate Using Gas-Liquid Chromatography:	https://www.doi.org/10.1021/acs.jced.8b00080
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Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 4-(2-methoxyethyl)-4-methylmorpholinium trifluorotris(perfluoroethyl)phosphate:	https://www.doi.org/10.1016/j.jct.2012.05.017
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(2-hydroxyethyl)-3-methylimidazolium trifluorotris(perfluoroethyl)phosphate:	https://www.doi.org/10.1016/j.jct.2013.05.008

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Activity coefficients at infinite dilution of organic solutes in N-alkylpyridinium bis(trifluoromethylsulfonyl)imide ([CnPY][NTf2], n = 2, 4, 5) using gas liquid chromatography:	https://www.doi.org/10.1016/j.jct.2010.06.009
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Activity coefficients at infinite dilution of organic solutes in the ionic liquid, methyl(trioctyl)ammonium thiosalicylate, [N1888][TS] by gas liquid chromatography at T = (303.15, 313.15, and 323.15) K:	https://www.doi.org/10.1016/j.jct.2010.12.020
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Activity coefficients at infinite dilution, physicochemical and thermodynamic properties of organic solutes and water in 1-butyl-1-methylpyrrolidinium tricyanomethanide:	https://www.doi.org/10.1016/j.jct.2015.05.022
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Activity Coefficients at Infinite Dilution of Organic Solutes in 1-Ethyl-3-methylimidazolium Tris(pentafluoroethyl)trifluorophosphate [EMIM][FAP] Using Gas-Liquid Chromatography:	https://www.doi.org/10.1021/je9008443

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility