1-Octyne

Other names: HEXYLACETYLENE
Octyne-1
oct-1-yne
Inchi: InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h1H,4-8H2,2H3
InchiKey: UMIPWJGWASORKV-UHFFFAOYSA-N
Formula: C8H14
SMILES: C#CCCCCCC
Mol. weight [g/mol]: 110.20
CAS: 629-05-0

Physical Properties

Property code	Value	Unit	Source
gf	239.55	kJ/mol	Joback Method
hf	80.70 ± 3.60	kJ/mol	NIST Webbook
hfus	19.45	kJ/mol	Joback Method
hvap	42.30 ± 0.10	kJ/mol	NIST Webbook
hvap	42.34	kJ/mol	NIST Webbook
ie	9.95 ± 0.02	eV	NIST Webbook
log10ws	-3.66		Aqueous Solubility Prediction Method
log10ws	-3.66		Estimated Solubility Method
logp	2.590		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
rinpol	784.50		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	785.80		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	783.52		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	783.52		NIST Webbook
rinpol	783.60		NIST Webbook

rinpol	787.50		NIST Webbook
rinpol	788.10		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	784.00		NIST Webbook
ripol	1031.00		NIST Webbook
ripol	1047.10		NIST Webbook
ripol	1034.00		NIST Webbook
ripol	1036.00		NIST Webbook
tb	372.56	K	Joback Method
tc	547.48	K	Joback Method
tf	194.15 ± 1.50	K	NIST Webbook
tf	193.65 ± 0.30	K	NIST Webbook
tf	200.38	K	Aqueous Solubility Prediction Method
tf	193.67 ± 0.10	K	NIST Webbook
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.74	J/mol×K	372.56	Joback Method
cpg	219.42	J/mol×K	401.71	Joback Method
cpg	230.61	J/mol×K	430.87	Joback Method
cpg	241.34	J/mol×K	460.02	Joback Method
cpg	251.62	J/mol×K	489.17	Joback Method
cpg	261.46	J/mol×K	518.33	Joback Method
cpg	270.87	J/mol×K	547.48	Joback Method
hvapt	35.83	kJ/mol	399.40	NIST Webbook
hvapt	38.50	kJ/mol	378.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.39482e+01
Coeff. B	-3.12653e+03
Coeff. C	-6.42400e+01
Temperature range (K), min.	293.11
Temperature range (K), max.	426.24

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-2.39993e+00
Coeff. B	-4.34412e+03
Coeff. C	3.22566e+00
Coeff. D	-8.94889e-06
Temperature range (K), min.	357.15
Temperature range (K), max.	400.15

Sources

Activity coefficients at infinite dilution measurements for organic solutes and water in the 1-hexyloxymethyl-3-methyl-imidazolium and 1,3-dihexyloxymethyl-imidazolium bis(trifluoromethylsulfonyl)imide ionic liquids	https://www.doi.org/10.1016/j.fluid.2009.08.017
Activity coefficients at infinite dilution measurements for organic solutes in the ionic liquid bis(trifluoromethylsulfonyl)imide using g.l.c. at T = (298.15, 313.15, and 333.15) K	https://www.doi.org/10.1016/j.jct.2005.03.014
Separation of binary mixtures based on limiting activity coefficients data using new ionic liquid for alcohol extraction and investigation of functions:	https://www.doi.org/10.1016/j.fluid.2017.12.029
Limiting activity coefficients:	https://www.doi.org/10.1016/j.fluid.2018.07.028
Activity coefficients at infinite dilution of organic solutes in diethylene glycol and triethylene glycol from gas-liquid chromatography:	https://www.doi.org/10.1016/j.jct.2013.05.011
Thermodynamics and limiting activity coefficients measurements for organic solutes and water in the ionic liquid 1-dodecyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1016/j.jct.2016.08.008
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Activity coefficients at infinite dilution measurements for organic solutes in 4-(2-methoxyethyl)-4-methylmorpholinium bis(trifluoromethylsulfonyl)imide using GLC at T = (328.15, 333.15, 338.15, and 343.15) K:	https://www.doi.org/10.1016/j.fluid.2008.10.008
Screening of environmental friendly ionic liquid as a solvent for the different types of separations problem: Insight from activity coefficients at infinite dilution measurement using gas-liquid chromatography technique:	https://www.doi.org/10.1016/j.jct.2015.08.017
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
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McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Gas liquid chromatography measurements of activity coefficients at infinite dilution of various organic solutes and water in tri-iso-butylmethylphosphonium tosylate ionic liquid:	https://www.doi.org/10.1016/j.jct.2010.01.004
Infinite dilution activity coefficients, specific retention volumes and solvation thermodynamics	https://www.doi.org/10.1016/j.fluid.2006.07.015
Ammonium ionic liquids in extraction of bio-butan-1-ol from water phase using activity coefficients at infinite dilution:	https://www.doi.org/10.1016/j.fluid.2018.09.024
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
Activity coefficients at infinite dilution measurements for organic solutes in the ionic liquid	https://www.doi.org/10.1016/j.jct.2008.04.002
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid trihexyltetradecylphosphonium bis(2,4,4-trimethylpentyl)-phosphinate using GLC at T = (303.15, 308.15, 313.15, and 318.15) K	https://www.doi.org/10.1016/j.jct.2012.08.016
Measurements of activity coefficients at infinite dilution for organic solutes and water in the 1-methylpiperidinium liquid	https://www.doi.org/10.1016/j.jct.2011.11.025
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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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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Infinite Dilution Activity Coefficients for Trihexyltetradecyl Phosphonium Ionic Liquids: Measurements and COSMO-RS Prediction:	https://www.doi.org/10.1021/je0602925
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Measurements of activity coefficients at infinite dilution for organic solutes and water in the ionic liquid [illegible] tricyanomethanide:	https://www.doi.org/10.1016/j.jct.2013.07.004
Activity coefficients at infinite dilution measurements for organic solutes in the ionic liquid 1-butyl-3-methylimidazolium 2-(2-methoxyethoxy) ethyl sulfate using [illegible]	https://www.doi.org/10.1016/j.jct.2005.01.015
Activity coefficients at infinite dilution of organic solutes in the ionic liquid [illegible]	https://www.doi.org/10.1016/j.jct.2009.12.004
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Activity Coefficients at Infinite Dilution of Organic Solutes and Water in Tributylethylphosphonium Diethylphosphate Using Gas–Liquid Chromatography: Thermodynamic Properties of Mixtures Containing Ionic Liquids:	https://www.doi.org/10.1021/acs.jced.5b00980
Thermodynamics and activity coefficients at infinite dilution for organic solutes [illegible]	https://www.doi.org/10.1016/j.fluid.2018.06.013
Measurements of activity coefficients at infinite dilution of organic solutes [illegible] 1-propyl-1-methylpiperidinium bis(trifluoromethylsulfonyl)imide ionic liquid using g.l.c.:	https://www.doi.org/10.1016/j.jct.2010.05.017
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
Tetramethylammonium chloride : glycerol deep eutectic solvent as separation agent for organic liquid mixtures: Assessment from experimental limiting activity coefficients:	https://www.doi.org/10.1016/j.fluid.2018.06.003
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
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
Determination of Activity Coefficients at Infinite Dilution of Solutes in the Ionic Liquid 1-Hexyl-3-methylimidazolium Tetrafluoroborate Using Gas-Liquid Chromatography at the Temperatures 298.15 K and 323.15 K:	https://www.doi.org/10.1021/je030187k
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Activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-ethyl-3-methylimidazolium tetracyanoborate [EMIM][TCB] using gas-liquid chromatography:	https://www.doi.org/10.1016/j.jct.2010.02.006
Determination of activity coefficients at infinite dilution of organic solutes in [illegible]	https://www.doi.org/10.1016/j.fluid.2005.04.021
Activity coefficients at infinite dilution of organic solutes in the ionic liquid trihexyl(tetradecyl)phosphonium tris(pentafluoroethyl)trifluorophosphate [illegible]	https://www.doi.org/10.1016/j.jct.2009.07.010
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(2-methoxyethyl)-1-methylpiperidinium bis(trifluoromethylsulfonyl)-amide:	https://www.doi.org/10.1016/j.jct.2012.01.019
Measurement of activity coefficients at infinite dilution of organic solutes in the ionic liquid [illegible] 2-(2-methoxyethoxy) ethylsulfate at T = [illegible] K	https://www.doi.org/10.1016/j.jct.2013.10.017
Activity coefficients at infinite dilution for solutes in the [illegible]	https://www.doi.org/10.1016/j.jct.2009.08.012
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
Activity coefficients at infinite dilution [illegible] tetradecyl-phosphonium [illegible]	https://www.doi.org/10.1016/j.jct.2018.01.003
Activity coefficients at infinite dilution measurements for organic solutes and water in the ionic liquid 1-butyl-1-methylpyrrolidinium trifluoromethanesulfonate using GLC:	https://www.doi.org/10.1016/j.fluid.2009.01.011
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Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamics and activity coefficients at infinite dilution measurements for organic solutes and water in the ionic liquid 1-butyl-1-methylpyrrolidinium tetracyanoborate:	https://www.doi.org/10.1016/j.jct.2011.06.007
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(3-hydroxypropyl)pyridinium bis(trifluoromethylsulfonyl)-amide:	https://www.doi.org/10.1016/j.jct.2011.04.018
Activity coefficients at infinite dilution measurements for organic solutes and water in the ionic liquid 1-ethyl-3-methylimidazolium tetracyanoborate:	https://www.doi.org/10.1016/j.jct.2011.02.012
Separation of aliphatic from aromatic hydrocarbons and sulphur compounds from fuel based on measurements of activity coefficients at infinite dilution [illegible]	https://www.doi.org/10.1016/j.jct.2016.07.017
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid N,N-diethyl-N-methyl-N-(2-methoxy-ethyl)ammonium [illegible]	https://www.doi.org/10.1016/j.jct.2013.01.007
Determination of Activity Coefficients at Infinite Dilution of Solutes in the Ionic Liquid 1-Butyl-3-methylimidazolium Octyl Sulfate Using Gas-Liquid Chromatography at a Temperature of 298.15 K, 313.15 K, or 328.15 K:	https://www.doi.org/10.1021/je0500375
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[illegible] separation based on activity coefficients at infinite dilution of various solutes in 1-allyl-3-methylimidazolium bis{(trifluoromethyl)sulfonyl}imide ionic liquid:	https://www.doi.org/10.1016/j.jct.2016.06.028
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(2-methoxyethyl)-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)-amide:	https://www.doi.org/10.1016/j.jct.2012.03.015
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KDB	https://www.cheric.org/files/research/kdb/mol/mol428.mol
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Activity coefficients at infinite dilution measurements for organic solutes and ...	https://www.doi.org/10.1016/j.jct.2008.12.005
Activity coefficients at infinite dilution measurements for organic solutes and ...	https://www.doi.org/10.1016/j.jct.2009.06.011
Measurements of activity coefficients at infinite dilution of aromatic and ...	https://www.doi.org/10.1016/j.jct.2008.12.018
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Activity coefficients at infinite dilution of organic solvents and water in ...	https://www.doi.org/10.1016/j.fluid.2016.02.004
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Determination of Activity Coefficients at Infinite Dilution of Polar and ... 1-Ethyl-3-methyl- imidazolium Bis(trifluoromethylsulfonyl) imidate ...	https://www.doi.org/10.1021/je0498107
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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

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