1-Nonyne

Other names: 1-C9H16
heptylacetylene
non-1-yne
Inchi: InChI=1S/C9H16/c1-3-5-7-9-8-6-4-2/h1H,4-9H2,2H3
InchiKey: OSSQSXOTMIGBCF-UHFFFAOYSA-N
Formula: C9H16
SMILES: C#CCCCCCCC
Mol. weight [g/mol]: 124.22
CAS: 3452-09-3

Physical Properties

Property code	Value	Unit	Source
af	0.3820		KDB
gf	247.97	kJ/mol	Joback Method
hcg	5856.76	kJ/mol	KDB
hcn	5505.308	kJ/mol	KDB
hf	62.30 ± 3.00	kJ/mol	NIST Webbook
hfus	22.04	kJ/mol	Joback Method
hvap	35.49	kJ/mol	Joback Method
ie	9.93 ± 0.02	eV	NIST Webbook
log10ws	-4.24		Estimated Solubility Method
log10ws	-4.24		Aqueous Solubility Prediction Method
logp	2.980		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2670.00	kPa	KDB
rinpol	884.00		NIST Webbook
rinpol	885.30		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	887.90		NIST Webbook
rinpol	884.00		NIST Webbook

rinpol	888.50		NIST Webbook
ripol	1135.00		NIST Webbook
ripol	1132.00		NIST Webbook
ripol	1134.00		NIST Webbook
ripol	1147.90		NIST Webbook
ripol	1133.00		NIST Webbook
tb	424.00	K	KDB
tc	610.80	K	KDB
tf	223.00	K	KDB
vc	0.501	m3/kmol	KDB
zc	0.2636610		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.83	J/mol×K	395.44	Joback Method
cpg	258.73	J/mol×K	424.49	Joback Method
cpg	271.09	J/mol×K	453.53	Joback Method
cpg	282.94	J/mol×K	482.58	Joback Method
cpg	294.28	J/mol×K	511.63	Joback Method
cpg	305.15	J/mol×K	540.67	Joback Method
cpg	315.54	J/mol×K	569.72	Joback Method
hvapt	45.60 ± 0.20	kJ/mol	392.00	NIST Webbook
hvapt	42.70 ± 0.20	kJ/mol	392.00	NIST Webbook
hvapt	39.70 ± 0.30	kJ/mol	392.00	NIST Webbook
hvapt	36.40 ± 0.50	kJ/mol	392.00	NIST Webbook
rfi	1.41950		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53731e+01
Coeff. B	-3.92375e+03
Coeff. C	-5.90110e+01
Temperature range (K), min.	319.11
Temperature range (K), max.	448.98

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.44707e+01
Coeff. B	-8.15030e+03
Coeff. C	-1.19523e+01
Coeff. D	9.23357e-06
Temperature range (K), min.	323.15
Temperature range (K), max.	610.81

Sources

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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3452093&Units=SI
Activity coefficients at infinite dilution for solutes in the trioctylmethylammonium bis(trifluoromethylsulfonyl)imide ionic liquid using gas liquid chromatography:	https://www.doi.org/10.1016/j.jct.2009.08.012
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Measurement of activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-ethyl-3-methylimidazolium 2-(2-methoxyethoxy) ethylsulfate at T = (298.15, 313.15, 323.15 and 333.15) K using gas + liquid chromatography:	https://www.doi.org/10.1016/j.jct.2013.10.017
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-ethyl-3-methylimidazolium hexafluorophosphate using gas liquid chromatography at T = (313.15, 333.15, and 353.15) K:	https://www.doi.org/10.1016/j.jct.2012.01.004
Activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-ethyl-3-methylimidazolium tetrafluoroborate using gas liquid chromatography at T = (313.15, 333.15, and 353.15) K:	https://www.doi.org/10.1016/j.jct.2010.12.005
KDB Vapor Pressure Database:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=432
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
KDB:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Infinite dilution activity coefficients, specific retention volumes and solvation thermodynamics of organic solutes in the ionic liquid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide using gas-liquid chromatography at T = (313.15, 333.15, and 353.15) K:	https://www.cheric.org/files/research/kdb/mol/mol432.mol
Activity coefficients at infinite dilution of organic solutes in the ionic liquid trihexyltetradecylphosphonium bis(trifluoromethylsulfonyl)imide using gas-liquid chromatography at T = (313.15, 333.15, and 353.15) K:	https://www.doi.org/10.1016/j.fluid.2006.07.015
Aqueous Solubility Prediction Method:	https://www.doi.org/10.1016/j.jct.2013.05.030
Screening of environmental friendly ionic liquids as a solvent for the different types of separations problem:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Thermodynamic parameters and insight from activity coefficients at infinite dilution measurement using (gas + liquid) chromatography technique:	https://www.doi.org/10.1016/j.jct.2015.08.017
Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
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
zc:	Critical Compressibility