1-Heptyne

Other names:	AMYLACETYLENE
	hept-1-yne
	n-C5H11C«equiv»CH
	n-C5H11CÂ«equivÂ»CH
Inchi:	InChI=1S/C7H12/c1-3-5-7-6-4-2/h1H,4-7H2,2H3
InchiKey:	YVXHZKKCZYLQOP-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	C#CCCCCC
Mol. weight [g/mol]:	96.17
CAS:	628-71-7

Physical Properties

Property code	Value	Unit	Source
af	0.2930		KDB
chl	-4570.60	kJ/mol	NIST Webbook
gf	231.13	kJ/mol	Joback Method
hcg	4542.99	kJ/mol	KDB
hcn	4279.395	kJ/mol	KDB
hf	103.80 ± 2.60	kJ/mol	NIST Webbook
hf	101.70	kJ/mol	NIST Webbook
hfl	101.10 ± 4.00	kJ/mol	NIST Webbook
hfl	-62.80	kJ/mol	NIST Webbook
hfus	16.86	kJ/mol	Joback Method
hvap	31.03	kJ/mol	Joback Method
ie	10.04 ± 0.01	eV	NIST Webbook
log10ws	-3.01		Estimated Solubility Method
log10ws	-3.01		Aqueous Solubility Prediction Method
logp	2.200		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3300.00	kPa	KDB
rinpol	686.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	687.10		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	684.00		NIST Webbook

rinpol	685.30		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	687.30		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	688.20		NIST Webbook
rinpol	687.00		NIST Webbook
ripol	947.00		NIST Webbook
ripol	938.00		NIST Webbook
ripol	934.00		NIST Webbook
ripol	929.00		NIST Webbook
tb	373.15 ± 3.00	K	NIST Webbook
tb	372.90 ± 1.50	K	NIST Webbook
tb	360.15	K	NIST Webbook
tb	373.15 ± 1.50	K	NIST Webbook
tb	373.15 ± 1.50	K	NIST Webbook
tb	373.15 ± 1.50	K	NIST Webbook
tb	371.15 ± 1.50	K	NIST Webbook
tb	372.65 ± 1.50	K	NIST Webbook
tb	373.75 ± 1.50	K	NIST Webbook
tb	379.15 ± 5.00	K	NIST Webbook
tb	372.65 ± 1.50	K	NIST Webbook
tb	371.65 ± 1.00	K	NIST Webbook
tb	371.65 ± 1.50	K	NIST Webbook
tb	371.15 ± 0.50	K	NIST Webbook
tb	372.15 ± 1.50	K	NIST Webbook
tb	371.75 ± 1.50	K	NIST Webbook
tb	371.65 ± 1.00	K	NIST Webbook
tb	372.15 ± 1.50	K	NIST Webbook
tb	372.93 ± 0.20	K	NIST Webbook
tb	372.89 ± 0.40	K	NIST Webbook
tb	372.89 ± 0.30	K	NIST Webbook
tb	372.65 ± 2.00	K	NIST Webbook
tb	371.65 ± 2.00	K	NIST Webbook
tb	374.00 ± 2.00	K	NIST Webbook

tb	371.15 ± 1.50	K	NIST Webbook
tb	372.99 ± 0.50	K	NIST Webbook
tb	372.90	K	NIST Webbook
tb	372.50 ± 0.50	K	NIST Webbook
tb	372.15 ± 2.00	K	NIST Webbook
tb	372.15 ± 2.00	K	NIST Webbook
tb	372.90	K	KDB
tb	371.15 ± 1.50	K	NIST Webbook
tb	372.15 ± 2.00	K	NIST Webbook
tb	372.65 ± 0.70	K	NIST Webbook
tc	559.70	K	KDB
tf	192.15 ± 1.50	K	NIST Webbook
tf	192.22 ± 0.10	K	NIST Webbook
tf	192.10 ± 0.50	K	NIST Webbook
tf	192.00	K	KDB
vc	0.390	m3/kmol	KDB
zc	0.2762040		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.06	J/mol×K	349.68	Joback Method
cpg	182.39	J/mol×K	378.88	Joback Method
cpg	192.30	J/mol×K	408.09	Joback Method
cpg	201.79	J/mol×K	437.29	Joback Method
cpg	210.88	J/mol×K	466.49	Joback Method
cpg	219.59	J/mol×K	495.70	Joback Method
cpg	227.93	J/mol×K	524.90	Joback Method
hvapt	37.90	kJ/mol	354.50	NIST Webbook
rfi	1.40610		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38643e+01
Coeff. B	-2.91233e+03

Coeff. C	-5.79460e+01
Temperature range (K), min.	272.46
Temperature range (K), max.	398.46

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.20864e+01
Coeff. B	-6.66117e+03
Coeff. C	-1.02999e+01
Coeff. D	9.86822e-06
Temperature range (K), min.	287.15
Temperature range (K), max.	559.69

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[illegible]	https://www.doi.org/10.1016/j.fluid.2019.03.023
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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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(2-methoxyethyl)-1-methylpiperidinium bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1016/j.jct.2012.08.016
Activity coefficients at infinite dilution of organic solutes in N-alkylpyridinium ionic liquid tris(perfluoroethyl)trifluorophosphate: liquid chromatography:	https://www.doi.org/10.1016/j.jct.2010.06.009
Activity coefficients at infinite dilution of aromatic 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

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
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
hfl:	Liquid phase 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