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	144.30 ± 2.10	kJ/mol	NIST Webbook
hf	144.40	kJ/mol	KDB
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 ± 0.01	eV	NIST Webbook
ie	10.05	eV	NIST Webbook
ie	10.10 ± 0.02	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	484.50		NIST Webbook
rinpol	484.40		NIST Webbook

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

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.31	J/mol×K	391.11	Joback Method
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	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

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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