2-Pentyne

Other names:	1-ETHYL-2-METHYLACETYLENE
	C2H5C«equiv»CCH3
	C2H5CÂ«equivÂ»CCH3
	ETHYLMETHYLACETYLENE
	pent-2-yne
Inchi:	InChI=1S/C5H8/c1-3-5-4-2/h3H2,1-2H3
InchiKey:	NKTDTMONXHODTI-UHFFFAOYSA-N
Formula:	C5H8
SMILES:	CC#CCC
Mol. weight [g/mol]:	68.12
CAS:	627-21-4

Physical Properties

Property code	Value	Unit	Source
af	0.1860		KDB
affp	810.20	kJ/mol	NIST Webbook
basg	778.00	kJ/mol	NIST Webbook
gf	194.02	kJ/mol	Joback Method
hcg	3208.92	kJ/mol	KDB
hcn	3032.856	kJ/mol	KDB
hf	128.90 ± 2.10	kJ/mol	NIST Webbook
hfus	11.83	kJ/mol	Joback Method
hvap	30.80	kJ/mol	NIST Webbook
ie	9.44 ± 0.02	eV	NIST Webbook
ie	9.44 ± 0.01	eV	NIST Webbook
log10ws	-1.71		Crippen Method
logp	1.420		Crippen Method
mcvol	72.710	ml/mol	McGowan Method
pc	4230.00	kPa	KDB
rinpol	547.00		NIST Webbook
rinpol	566.00		NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	566.00		NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	570.00		NIST Webbook
rinpol	548.00		NIST Webbook

rinpol	548.00		NIST Webbook
rinpol	548.00		NIST Webbook
rinpol	579.00		NIST Webbook
tb	329.05 ± 0.50	K	NIST Webbook
tb	328.90 ± 1.50	K	NIST Webbook
tb	325.65 ± 3.00	K	NIST Webbook
tb	328.65 ± 0.40	K	NIST Webbook
tb	328.65 ± 1.50	K	NIST Webbook
tb	330.15 ± 2.00	K	NIST Webbook
tb	329.15 ± 0.00	K	NIST Webbook
tb	328.15 ± 1.50	K	NIST Webbook
tb	328.20 ± 0.80	K	NIST Webbook
tb	328.40 ± 1.00	K	NIST Webbook
tb	328.15 ± 2.00	K	NIST Webbook
tb	329.35 ± 0.50	K	NIST Webbook
tb	329.22 ± 0.40	K	NIST Webbook
tb	329.22 ± 0.30	K	NIST Webbook
tb	329.22 ± 0.40	K	NIST Webbook
tb	328.90 ± 1.00	K	NIST Webbook
tb	329.27 ± 0.20	K	NIST Webbook
tb	329.17 ± 0.30	K	NIST Webbook
tb	329.10 ± 2.00	K	NIST Webbook
tb	329.00	K	NIST Webbook
tb	329.20	K	KDB
tb	329.30	K	NIST Webbook
tc	522.00	K	KDB
tf	164.00	K	KDB
tf	163.70 ± 0.20	K	NIST Webbook
tf	172.00 ± 2.00	K	NIST Webbook
tf	163.82 ± 0.50	K	NIST Webbook
tf	163.82 ± 0.10	K	NIST Webbook
vc	0.278	m3/kmol	KDB
zc	0.2704560		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	106.77	J/mol×K	322.80	Joback Method
cpg	114.10	J/mol×K	354.30	Joback Method
cpg	121.18	J/mol×K	385.80	Joback Method
cpg	128.02	J/mol×K	417.31	Joback Method

cpg	134.61	J/mol×K	448.81	Joback Method
cpg	140.96	J/mol×K	480.31	Joback Method
cpg	147.08	J/mol×K	511.81	Joback Method
hvapt	29.25	kJ/mol	329.20	KDB
hvapt	33.10	kJ/mol	284.50	NIST Webbook
rfi	1.40090		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37271e+01
Coeff. B	-2.54589e+03
Coeff. C	-4.97730e+01
Temperature range (K), min.	239.21
Temperature range (K), max.	352.29

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.65428e+01
Coeff. B	-6.17875e+03
Coeff. C	-9.29145e+00
Coeff. D	6.47742e-06
Temperature range (K), min.	240.15
Temperature range (K), max.	521.99

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol405.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C627214&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=405

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility