Acetylene

Other names:	ACETYLEN
	C2H2
	ETHYNE
	Ethine
	NARCYLEN
	UN 1001
	Vinylene
Inchi:	InChI=1S/C2H2/c1-2/h1-2H
InchiKey:	HSFWRNGVRCDJHI-UHFFFAOYSA-N
Formula:	C2H2
SMILES:	C#C
Mol. weight [g/mol]:	26.04
CAS:	74-86-2

Physical Properties

Property code	Value	Unit	Source
af	0.1900		KDB
affp	641.40	kJ/mol	NIST Webbook
aigt	578.15	K	KDB
basg	616.70	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
fll	2.50	% in Air	KDB
flu	80.00	% in Air	KDB
gf	209.30	kJ/mol	KDB
gyrad	1.0950		KDB
hf	227.40 ± 0.80	kJ/mol	NIST Webbook
hf	226.70 ± 0.79	kJ/mol	NIST Webbook
hf	226.90	kJ/mol	KDB
hfus	3.76	kJ/mol	Joback Method
hvap	17.61	kJ/mol	Joback Method
ie	11.37 ± 0.05	eV	NIST Webbook
ie	11.40	eV	NIST Webbook
ie	11.40 ± 0.10	eV	NIST Webbook
ie	11.40 ± 0.10	eV	NIST Webbook
ie	11.40 ± 0.02	eV	NIST Webbook
ie	11.30	eV	NIST Webbook
ie	11.40	eV	NIST Webbook

ie	11.40 ± 0.00	eV	NIST Webbook
ie	11.39 ± 0.01	eV	NIST Webbook
ie	11.40 ± 0.01	eV	NIST Webbook
ie	11.40	eV	NIST Webbook
ie	11.39 ± 0.02	eV	NIST Webbook
ie	11.40	eV	NIST Webbook
ie	11.39 ± 0.05	eV	NIST Webbook
ie	11.41 ± 0.01	eV	NIST Webbook
ie	11.40 ± 0.01	eV	NIST Webbook
ie	11.40 ± 0.01	eV	NIST Webbook
ie	11.40 ± 0.00	eV	NIST Webbook
ie	11.40 ± 0.02	eV	NIST Webbook
ie	11.41 ± 0.01	eV	NIST Webbook
ie	11.41 ± 0.01	eV	NIST Webbook
ie	11.40	eV	NIST Webbook
ie	11.41	eV	NIST Webbook
ie	11.49	eV	NIST Webbook
ie	11.43	eV	NIST Webbook
ie	11.41 ± 0.01	eV	NIST Webbook
ie	11.20 ± 0.10	eV	NIST Webbook
ie	11.39 ± 0.01	eV	NIST Webbook
ie	11.40 ± 0.00	eV	NIST Webbook
log10ws	0.29		Estimated Solubility Method
log10ws	0.29		Aqueous Solubility Prediction Method
logp	0.249		Crippen Method
mcvol	30.440	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=1)		KDB
nfpas	%!d(float64=3)		KDB
pc	6138.00	kPa	KDB
pc	6138.00 ± 10.00	kPa	NIST Webbook
pt	128.25 ± 0.39	kPa	NIST Webbook
rhoc	231.99 ± 0.26	kg/m3	NIST Webbook
rinpol	157.00		NIST Webbook
rinpol	156.00		NIST Webbook
rinpol	195.00		NIST Webbook
rinpol	182.00		NIST Webbook
rinpol	176.00		NIST Webbook
rinpol	156.00		NIST Webbook
rinpol	182.00		NIST Webbook
rinpol	155.00		NIST Webbook
rinpol	165.00		NIST Webbook
rinpol	165.00		NIST Webbook

rinpol	155.00		NIST Webbook
rinpol	156.00		NIST Webbook
tb	188.43	K	KDB
tb	189.00	K	NIST Webbook
tb	189.60 ± 0.30	K	NIST Webbook
tc	308.30 ± 0.10	K	NIST Webbook
tc	309.70 ± 0.60	K	NIST Webbook
tc	308.30	K	KDB
tc	308.35	K	NIST Webbook
tc	308.66	K	NIST Webbook
tf	171.65 ± 0.50	K	NIST Webbook
tf	191.40 ± 1.00	K	NIST Webbook
tf	191.65 ± 0.50	K	NIST Webbook
tf	192.40	K	KDB
tf	192.40	K	Aqueous Solubility Prediction Method
tt	192.40 ± 0.50	K	NIST Webbook
tt	191.35 ± 0.30	K	NIST Webbook
vc	0.112	m3/kmol	NIST Webbook
vc	0.112	m3/kmol	KDB
vc	0.113	m3/kmol	NIST Webbook
zc	0.2686640		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	43.90	J/mol×K	291.84	Joback Method
cpg	45.72	J/mol×K	316.99	Joback Method
cpg	47.41	J/mol×K	342.14	Joback Method
cpg	37.58	J/mol×K	216.40	Joback Method
cpg	39.83	J/mol×K	241.55	Joback Method
cpg	41.94	J/mol×K	266.70	Joback Method
cpg	48.98	J/mol×K	367.29	Joback Method
hfust	3.76	kJ/mol	192.40	NIST Webbook
hfust	3.76	kJ/mol	192.40	NIST Webbook
hfust	2.54	kJ/mol	142.70	NIST Webbook
hsubt	25.20	kJ/mol	172.00	NIST Webbook
hsubt	22.70	kJ/mol	159.50	NIST Webbook
hsubt	22.10	kJ/mol	129.00	NIST Webbook
hsubt	23.50	kJ/mol	121.50	NIST Webbook

hsubt	21.80	kJ/mol	162.00	NIST Webbook
hvapt	17.00	kJ/mol	214.00	NIST Webbook
hvapt	16.40	kJ/mol	261.50	NIST Webbook
hvapt	16.80	kJ/mol	200.00	NIST Webbook
hvapt	16.67	kJ/mol	192.40	KDB
hvapt	16.30	kJ/mol	283.00	NIST Webbook
hvapt	16.70	kJ/mol	250.00	NIST Webbook
hvapt	16.70	kJ/mol	208.50	NIST Webbook
rhol	615.00	kg/m3	189.00	KDB
sfust	19.50	J/mol×K	192.40	NIST Webbook
sfust	17.80	J/mol×K	142.70	NIST Webbook
srf	0.02	N/m	203.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.76267e+01
Coeff. B	-2.32926e+03
Coeff. C	-1.02910e+01
Temperature range (K), min.	144.63
Temperature range (K), max.	268.30

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.88347e+01
Coeff. B	-3.71141e+03
Coeff. C	-1.05984e+01
Coeff. D	2.80537e-05
Temperature range (K), min.	189.00
Temperature range (K), max.	308.32

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=399

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=399
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Solubility of Acetylene in Alcohols and Ketones:	https://www.doi.org/10.1021/acs.jced.8b00126
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74862&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol399.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
gf:	Standard Gibbs free energy of formation
gyrad:	Radius of Gyration
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pt:	Triple Point Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density

rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter