2-Butyne

Other names:	But-2-yne
	CH3C«equiv»CCH3
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	CROTONYLENE
	Dimethylacetylene
	UN 1144
Inchi:	InChI=1S/C4H6/c1-3-4-2/h1-2H3
InchiKey:	XNMQEEKYCVKGBD-UHFFFAOYSA-N
Formula:	C4H6
SMILES:	CC#CC
Mol. weight [g/mol]:	54.09
CAS:	503-17-3

Physical Properties

Property code	Value	Unit	Source
af	0.1305		KDB
affp	775.80	kJ/mol	NIST Webbook
basg	745.10	kJ/mol	NIST Webbook
chg	-2576.70 ± 0.96	kJ/mol	NIST Webbook
dm	0.80	debye	KDB
gf	185.60	kJ/mol	KDB
hcg	2550.94	kJ/mol	KDB
hcn	2418.896	kJ/mol	KDB
hf	146.40	kJ/mol	KDB
hf	148.00 ± 1.50	kJ/mol	NIST Webbook
hf	145.10 ± 1.00	kJ/mol	NIST Webbook
hfus	9.24	kJ/mol	Joback Method
hvap	26.70	kJ/mol	NIST Webbook
ie	9.59 ± 0.02	eV	NIST Webbook
ie	9.61	eV	NIST Webbook
ie	9.56 ± 0.01	eV	NIST Webbook
ie	9.59	eV	NIST Webbook
ie	9.56	eV	NIST Webbook
ie	9.79	eV	NIST Webbook
ie	9.58 ± 0.02	eV	NIST Webbook
log10ws	-1.29		Crippen Method
logp	1.030		Crippen Method

mcvol	58.620	ml/mol	McGowan Method
pc	5080.00	kPa	KDB
rinpol	466.00		NIST Webbook
rinpol	463.00		NIST Webbook
rinpol	463.00		NIST Webbook
rinpol	482.00		NIST Webbook
rinpol	482.00		NIST Webbook
rinpol	462.00		NIST Webbook
rinpol	473.00		NIST Webbook
rinpol	488.00		NIST Webbook
rinpol	478.00		NIST Webbook
rinpol	485.00		NIST Webbook
rinpol	463.00		NIST Webbook
sl	195.10	J/mol×K	NIST Webbook
tb	300.12	K	KDB
tc	488.70	K	KDB
tf	240.63 ± 0.30	K	NIST Webbook
tf	240.90 ± 0.20	K	NIST Webbook
tf	240.82 ± 0.20	K	NIST Webbook
tf	240.79	K	KDB
tf	240.50 ± 0.30	K	NIST Webbook
tf	240.83 ± 0.10	K	NIST Webbook
tt	240.93 ± 0.06	K	NIST Webbook
tt	240.80 ± 0.15	K	NIST Webbook
vc	0.221	m3/kmol	KDB
zc	0.2762980		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	84.56	J/mol×K	336.07	NIST Webbook
cpg	89.66	J/mol×K	369.46	NIST Webbook
cpl	124.14	J/mol×K	290.00	NIST Webbook
hfust	9.23	kJ/mol	240.93	NIST Webbook
hfust	9.25	kJ/mol	240.90	NIST Webbook
hfust	9.25	kJ/mol	240.90	NIST Webbook
hfust	9.23	kJ/mol	240.92	NIST Webbook
hsubt	37.40	kJ/mol	219.50	NIST Webbook
hvapt	26.95	kJ/mol	291.00	NIST Webbook
hvapt	29.00	kJ/mol	274.00	NIST Webbook
hvapt	26.90 ± 0.30	kJ/mol	291.00	NIST Webbook

hvapt	26.65	kJ/mol	300.10	KDB
hvapt	26.95	kJ/mol	291.00	NIST Webbook
hvapt	26.90 ± 0.10	kJ/mol	291.00	NIST Webbook
rfi	1.38930		298.15	KDB
rhol	691.00	kg/m3	293.00	KDB
sfust	38.33	J/mol×K	240.93	NIST Webbook
sfust	38.35	J/mol×K	240.92	NIST Webbook
srf	0.02	N/m	298.20	KDB
svapt	92.59	J/mol×K	291.00	NIST Webbook
svapt	92.59	J/mol×K	291.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36731e+01
Coeff. B	-2.08471e+03
Coeff. C	-6.98960e+01
Temperature range (K), min.	225.64
Temperature range (K), max.	319.22

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.50165e+01
Coeff. B	-4.55895e+03
Coeff. C	-4.44326e+00
Coeff. D	1.52939e-06
Temperature range (K), min.	240.00
Temperature range (K), max.	488.15

Sources

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol403.mol

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C503173&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=403
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

vc:	Critical Volume
zc:	Critical Compressibility