1-Butyne

Other names:	Butyne-1
	C2H5C«equiv»CH
	C2H5CÂ«equivÂ»CH
	ETHYLACETYLENE
	ETHYLETHYNE
	Ethyl acetylene, inhibited
	UN 2452
	but-1-yne
Inchi:	InChI=1S/C4H6/c1-3-4-2/h1H,4H2,2H3
InchiKey:	KDKYADYSIPSCCQ-UHFFFAOYSA-N
Formula:	C4H6
SMILES:	C#CCC
Mol. weight [g/mol]:	54.09
CAS:	107-00-6

Physical Properties

Property code	Value	Unit	Source
af	0.1182		KDB
chg	-2596.80 ± 0.84	kJ/mol	NIST Webbook
dm	0.80	debye	KDB
gf	202.20	kJ/mol	KDB
hcg	2572.53	kJ/mol	KDB
hcn	2440.527	kJ/mol	KDB
hf	165.30	kJ/mol	KDB
hf	166.10 ± 2.10	kJ/mol	NIST Webbook
hf	165.20 ± 0.88	kJ/mol	NIST Webbook
hfus	9.09	kJ/mol	Joback Method
hvap	23.79	kJ/mol	NIST Webbook
hvap	23.38	kJ/mol	NIST Webbook
hvap	23.70	kJ/mol	NIST Webbook
ie	10.18	eV	NIST Webbook
ie	10.20 ± 0.02	eV	NIST Webbook
ie	10.18 ± 0.01	eV	NIST Webbook
ie	10.18 ± 0.01	eV	NIST Webbook
ie	10.18	eV	NIST Webbook
ie	10.18 ± 0.01	eV	NIST Webbook

log10ws	-1.24		Aqueous Solubility Prediction Method
log10ws	-1.24		Estimated Solubility Method
logp	1.030		Crippen Method
mcvol	58.620	ml/mol	McGowan Method
pc	4600.00 ± 200.00	kPa	NIST Webbook
pc	4600.00	kPa	KDB
rhoc	259.63 ± 10.82	kg/m3	NIST Webbook
rinpol	385.00		NIST Webbook
rinpol	424.00		NIST Webbook
rinpol	414.00		NIST Webbook
rinpol	385.00		NIST Webbook
rinpol	385.00		NIST Webbook
rinpol	385.00		NIST Webbook
rinpol	385.00		NIST Webbook
rinpol	420.00		NIST Webbook
rinpol	424.00		NIST Webbook
rinpol	385.00		NIST Webbook
rinpol	417.00		NIST Webbook
rinpol	416.00		NIST Webbook
rinpol	408.00		NIST Webbook
sl	197.48	J/mol×K	NIST Webbook
tb	281.23	K	KDB
tc	440.00	K	KDB
tc	463.60	K	NIST Webbook
tc	440.00 ± 2.00	K	NIST Webbook
tf	147.28 ± 0.20	K	NIST Webbook
tf	147.43	K	KDB
tf	150.65 ± 0.60	K	NIST Webbook
tf	147.49 ± 0.20	K	NIST Webbook
tf	147.45	K	Aqueous Solubility Prediction Method
tf	147.39 ± 0.50	K	NIST Webbook
tf	147.49 ± 0.30	K	NIST Webbook
tt	147.41 ± 0.06	K	NIST Webbook
tt	147.45 ± 0.08	K	NIST Webbook
vc	0.208	m3/kmol	NIST Webbook
vc	0.208	m3/kmol	KDB
zc	0.2615360		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	96.68	J/mol×K	367.55	Joback Method
cpg	101.55	J/mol×K	396.38	Joback Method
cpg	106.22	J/mol×K	425.22	Joback Method
cpg	80.74	J/mol×K	281.04	Joback Method
cpg	86.28	J/mol×K	309.88	Joback Method
cpg	91.59	J/mol×K	338.71	Joback Method
cpg	110.68	J/mol×K	454.05	Joback Method
cpl	132.42	J/mol×K	280.00	NIST Webbook
hfust	6.03	kJ/mol	147.43	NIST Webbook
hfust	6.03	kJ/mol	147.40	NIST Webbook
hfust	6.03	kJ/mol	147.40	NIST Webbook
hvapt	26.00	kJ/mol	247.00	NIST Webbook
hvapt	25.80 ± 0.10	kJ/mol	263.00	NIST Webbook
hvapt	24.50 ± 0.10	kJ/mol	281.00	NIST Webbook
hvapt	24.98	kJ/mol	281.20	KDB
hvapt	24.52	kJ/mol	281.23	NIST Webbook
hvapt	24.52	kJ/mol	281.20	NIST Webbook
rhol	650.00	kg/m3	289.00	KDB
sfust	40.89	J/mol×K	147.43	NIST Webbook
srf	0.02	N/m	273.20	KDB
svapt	87.20	J/mol×K	281.23	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44978e+01
Coeff. B	-2.46519e+03
Coeff. C	-3.16930e+01
Temperature range (K), min.	205.17
Temperature range (K), max.	300.05

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.85412e+01
Coeff. B	-5.68731e+03
Coeff. C	-1.14326e+01
Coeff. D	1.25220e-05
Temperature range (K), min.	147.43
Temperature range (K), max.	443.20

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol402.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107006&Units=SI
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=402
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

af:	Acentric Factor
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
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
rhoc:	Critical density
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
zra:	Rackett Parameter