1,3-Butadiyne

Other names:	Biacetylene
	Biethynyl
	Butadiyne
	Diacetylene
	HC«equiv»CC«equiv»CH
	HCÂ«equivÂ»CCÂ«equivÂ»CH
	buta-1,3-diyne
Inchi:	InChI=1S/C4H2/c1-3-4-2/h1-2H
InchiKey:	LLCSWKVOHICRDD-UHFFFAOYSA-N
Formula:	C4H2
SMILES:	C#CC#C
Mol. weight [g/mol]:	50.06
CAS:	460-12-8

Physical Properties

Property code	Value	Unit	Source
affp	737.20	kJ/mol	NIST Webbook
basg	712.80	kJ/mol	NIST Webbook
gf	428.94	kJ/mol	Joback Method
hf	464.00	kJ/mol	NIST Webbook
hfus	12.07	kJ/mol	Joback Method
hvap	24.21	kJ/mol	Joback Method
ie	10.17 ± 0.01	eV	NIST Webbook
ie	10.18 ± 0.00	eV	NIST Webbook
ie	10.17	eV	NIST Webbook
ie	10.10 ± 0.10	eV	NIST Webbook
ie	10.17 ± 0.02	eV	NIST Webbook
ie	10.17	eV	NIST Webbook
ie	10.30	eV	NIST Webbook
log10ws	-1.09		Crippen Method
logp	0.253		Crippen Method
mcvol	50.020	ml/mol	McGowan Method
pc	5862.92	kPa	Joback Method
rinpol	430.00		NIST Webbook
rinpol	428.00		NIST Webbook
rinpol	445.00		NIST Webbook
rinpol	431.00		NIST Webbook

rinpol	428.00		NIST Webbook
tb	283.00 ± 1.50	K	NIST Webbook
tb	282.90 ± 2.00	K	NIST Webbook
tb	286.80 ± 2.00	K	NIST Webbook
tb	281.90 ± 2.00	K	NIST Webbook
tb	283.50	K	NIST Webbook
tb	283.65 ± 1.00	K	NIST Webbook
tc	457.28	K	Joback Method
tf	263.00 ± 2.00	K	NIST Webbook
tf	237.00 ± 3.00	K	NIST Webbook
tf	237.70 ± 2.50	K	NIST Webbook
vc	0.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	77.10	J/mol×K	364.22	Joback Method
cpg	79.79	J/mol×K	395.24	Joback Method
cpg	84.61	J/mol×K	457.28	Joback Method
cpg	82.29	J/mol×K	426.26	Joback Method
cpg	67.77	J/mol×K	271.16	Joback Method
cpg	71.10	J/mol×K	302.18	Joback Method
cpg	74.21	J/mol×K	333.20	Joback Method
hsubt	36.20	kJ/mol	211.00	NIST Webbook
hsubt	36.30	kJ/mol	211.00	NIST Webbook
hvapt	26.40	kJ/mol	236.50	NIST Webbook
hvapt	26.10	kJ/mol	260.00	NIST Webbook
hvapt	33.40	kJ/mol	211.00	NIST Webbook
hvapt	25.40	kJ/mol	234.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.29299e+01
Coeff. B	-1.73811e+03
Coeff. C	-7.48820e+01

Temperature range (K), min.	212.36
Temperature range (K), max.	303.03

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C460128&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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