1-Butyne, 3-methyl-

Other names:	(CH3)2CHC«equiv»CH
	(CH3)2CHCÂ«equivÂ»CH
	2-Methyl-3-butyne
	3-Methyl-1-butyne
	3-Methylbutyne
	3-methylbut-1-yne
	ISOPENTYNE
	ISOPROPYLACETYLENE
	Isopropyl acetylene
Inchi:	InChI=1S/C5H8/c1-4-5(2)3/h1,5H,2-3H3
InchiKey:	USCSRAJGJYMJFZ-UHFFFAOYSA-N
Formula:	C5H8
SMILES:	C#CC(C)C
Mol. weight [g/mol]:	68.12
CAS:	598-23-2

Physical Properties

Property code	Value	Unit	Source
af	0.1760		KDB
affp	814.90	kJ/mol	NIST Webbook
basg	787.80	kJ/mol	NIST Webbook
gf	211.85	kJ/mol	Joback Method
hcg	3221.09	kJ/mol	KDB
hcn	3045.073	kJ/mol	KDB
hf	136.40 ± 2.10	kJ/mol	NIST Webbook
hfus	8.16	kJ/mol	Joback Method
hvap	26.19	kJ/mol	Joback Method
ie	9.97	eV	NIST Webbook
ie	10.05 ± 0.01	eV	NIST Webbook
ie	10.05 ± 0.02	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.276		Crippen Method
mcvol	72.710	ml/mol	McGowan Method
pc	4210.00	kPa	KDB
rinpol	436.00		NIST Webbook
rinpol	471.00		NIST Webbook
tb	299.50	K	KDB

tc	476.00	K	KDB
tf	183.00	K	KDB
vc	0.272	m3/kmol	KDB
zc	0.2888070		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	108.12	J/mol×K	303.48	Joback Method
cpg	115.68	J/mol×K	333.29	Joback Method
cpg	122.92	J/mol×K	363.11	Joback Method
cpg	129.84	J/mol×K	392.92	Joback Method
cpg	136.46	J/mol×K	422.74	Joback Method
cpg	142.80	J/mol×K	452.55	Joback Method
cpg	148.85	J/mol×K	482.37	Joback Method
hvapt	26.15	kJ/mol	299.50	KDB
hvapt	30.20	kJ/mol	269.00	NIST Webbook
rfi	1.36950		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46392e+01
Coeff. B	-2.72830e+03
Coeff. C	-2.98900e+01
Temperature range (K), min.	219.99
Temperature range (K), max.	322.38

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.07703e+02
Coeff. B	-6.57589e+03
Coeff. C	-1.45180e+01
Coeff. D	1.81040e-05

Temperature range (K), min.	183.45
Temperature range (K), max.	463.20

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol406.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C598232&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=406
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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