1-Butyne, 3,3-dimethyl-

Other names:	(CH3)3CC«equiv»CH
	(CH3)3CCÂ«equivÂ»CH
	3,3,3-TRIMETHYLPROPYNE
	3,3-Dimethyl-1-Butyne
	3,3-Dimethylbutyne
	3,3-Dimethylbutyne-1
	TERT-BUTYLACETYLENE
	t-Butylacetylene
Inchi:	InChI=1S/C6H10/c1-5-6(2,3)4/h1H,2-4H3
InchiKey:	PPWNCLVNXGCGAF-UHFFFAOYSA-N
Formula:	C6H10
SMILES:	C#CC(C)(C)C
Mol. weight [g/mol]:	82.14
CAS:	917-92-0

Physical Properties

Property code	Value	Unit	Source
chl	-3868.10 ± 1.30	kJ/mol	NIST Webbook
chl	-3868.70 ± 2.40	kJ/mol	NIST Webbook
gf	225.55	kJ/mol	Joback Method
hf	107.00 ± 1.30	kJ/mol	NIST Webbook
hf	106.70	kJ/mol	NIST Webbook
hf	106.10	kJ/mol	NIST Webbook
hfl	77.90 ± 1.50	kJ/mol	NIST Webbook
hfl	77.80 ± 1.30	kJ/mol	NIST Webbook
hfl	78.50 ± 2.40	kJ/mol	NIST Webbook
hfus	6.86	kJ/mol	Joback Method
hvap	28.20	kJ/mol	NIST Webbook
hvap	29.20	kJ/mol	NIST Webbook
ie	9.92 ± 0.02	eV	NIST Webbook
ie	9.92 ± 0.01	eV	NIST Webbook
ie	10.67 ± 0.02	eV	NIST Webbook
ie	10.31 ± 0.04	eV	NIST Webbook
ie	10.21	eV	NIST Webbook
ie	9.80 ± 0.05	eV	NIST Webbook
ie	9.86	eV	NIST Webbook
log10ws	-1.89		Crippen Method

logp	1.666		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3777.68	kPa	Joback Method
rinpol	509.00		NIST Webbook
rinpol	467.00		NIST Webbook
rinpol	498.00		NIST Webbook
tb	323.57	K	Joback Method
tc	511.22	K	Joback Method
tf	194.94 ± 0.30	K	NIST Webbook
tf	192.00 ± 1.50	K	NIST Webbook
tf	192.00 ± 1.50	K	NIST Webbook
vc	0.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.60	J/mol×K	323.57	Joback Method
cpg	149.19	J/mol×K	354.85	Joback Method
cpg	159.18	J/mol×K	386.12	Joback Method
cpg	168.58	J/mol×K	417.40	Joback Method
cpg	177.44	J/mol×K	448.67	Joback Method
cpg	185.77	J/mol×K	479.95	Joback Method
cpg	193.60	J/mol×K	511.22	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35019e+01
Coeff. B	-2.32506e+03
Coeff. C	-4.89240e+01
Temperature range (K), min.	224.87
Temperature range (K), max.	332.80

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C917920&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol413.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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