2-Pentyne, 4,4-dimethyl-

Other names:	(tert-C4H9)C«equiv»CCH3
	(tert-C4H9)CÂ«equivÂ»CCH3
	1-TERT-BUTYL-PROPYNE
	4,4-Dimethyl-2-pentyne
	Propyne, 1-tert-butyl-
Inchi:	InChI=1S/C7H12/c1-5-6-7(2,3)4/h1-4H3
InchiKey:	FOALCTWKQSWRST-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	CC#CC(C)(C)C
Mol. weight [g/mol]:	96.17
CAS:	999-78-0

Physical Properties

Property code	Value	Unit	Source
gf	213.70	kJ/mol	Joback Method
hf	75.74	kJ/mol	Joback Method
hfus	9.59	kJ/mol	Joback Method
hvap	32.03	kJ/mol	Joback Method
ie	9.28 ± 0.01	eV	NIST Webbook
log10ws	-2.31		Crippen Method
logp	2.056		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
rinpol	612.00		NIST Webbook
rinpol	612.00		NIST Webbook
tb	356.10 ± 1.50	K	NIST Webbook
tb	355.65 ± 2.00	K	NIST Webbook
tb	356.15 ± 0.50	K	NIST Webbook
tb	356.00	K	NIST Webbook
tc	567.06	K	Joback Method
tf	190.78 ± 2.00	K	NIST Webbook
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.92	J/mol×K	365.33	Joback Method
cpg	185.20	J/mol×K	398.95	Joback Method
cpg	196.81	J/mol×K	432.57	Joback Method
cpg	207.81	J/mol×K	466.20	Joback Method
cpg	218.20	J/mol×K	499.82	Joback Method
cpg	228.03	J/mol×K	533.44	Joback Method
cpg	237.31	J/mol×K	567.06	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35592e+01
Coeff. B	-2.69400e+03
Coeff. C	-5.48390e+01
Temperature range (K), min.	257.83
Temperature range (K), max.	381.47

Sources

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/mol427.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C999780&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

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
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