

1-Pentyne, 3-methyl-

Other names:	3-Methyl-1-pentyne CH ₃ CH ₂ CH(CH ₃)C≡CH CH ₃ CH ₂ CH(CH ₃)C≡CH
Inchi:	InChI=1S/C6H10/c1-4-6(3)5-2/h1,6H,5H2,2-3H3
InchiKey:	PLHJCCHSCFNKCC-UHFFFAOYSA-N
Formula:	C ₆ H ₁₀
SMILES:	C#CC(C)CC
Mol. weight [g/mol]:	82.14
CAS:	922-59-8

Physical Properties

Property code	Value	Unit	Source
gf	220.27	kJ/mol	Joback Method
hf	119.45	kJ/mol	Joback Method
hfus	10.75	kJ/mol	Joback Method
hvap	28.42	kJ/mol	Joback Method
ie	9.98 ± 0.02	eV	NIST Webbook
ie	9.79 ± 0.05	eV	NIST Webbook
ie	9.97 ± 0.01	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	1.666		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
rinpol	539.00		NIST Webbook
rinpol	569.00		NIST Webbook
rinpol	539.00		NIST Webbook
tb	330.00	K	NIST Webbook
tb	330.85 ± 0.40	K	NIST Webbook
tc	505.86	K	Joback Method
tf	189.35	K	Joback Method
vc	0.328	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.67	J/mol×K	326.36	Joback Method
cpg	147.86	J/mol×K	356.28	Joback Method
cpg	156.66	J/mol×K	386.19	Joback Method
cpg	165.08	J/mol×K	416.11	Joback Method
cpg	173.13	J/mol×K	446.03	Joback Method
cpg	180.83	J/mol×K	475.94	Joback Method
cpg	188.19	J/mol×K	505.86	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37972e+01
Coeff. B	-2.56531e+03
Coeff. C	-5.06680e+01
Temperature range (K), min.	240.56
Temperature range (K), max.	352.98

Sources

KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=410
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C922598&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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