1,4-Pentadiene, 3-methyl-

Other names: 3-Methyl-1,4-pentadiene
3-methylpenta-1,4-diene
CH2=CHCH(CH3)CH=CH2
Inchi: InChI=1S/C6H10/c1-4-6(3)5-2/h4-6H,1-2H2,3H3
InchiKey: IKQUUYYDRTYXAP-UHFFFAOYSA-N
Formula: C6H10
SMILES: C=CC(C)C=C
Mol. weight [g/mol]: 82.14
CAS: 1115-08-8

Physical Properties

Property code	Value	Unit	Source
gf	172.88	kJ/mol	Joback Method
hf	78.41	kJ/mol	Joback Method
hfus	5.21	kJ/mol	Joback Method
hvap	27.22	kJ/mol	Joback Method
ie	9.40 ± 0.05	eV	NIST Webbook
log10ws	-1.80		Crippen Method
logp	1.994		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
rinpol	532.00		NIST Webbook
rinpol	532.00		NIST Webbook
rinpol	531.00		NIST Webbook
rinpol	534.00		NIST Webbook
rinpol	534.00		NIST Webbook
rinpol	546.00		NIST Webbook
tb	329.20	K	NIST Webbook
tb	322.77 ± 0.50	K	NIST Webbook
tc	504.04	K	Joback Method
tf	138.86	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.85	J/mol×K	329.60	Joback Method
cpg	142.48	J/mol×K	358.67	Joback Method
cpg	151.69	J/mol×K	387.75	Joback Method
cpg	160.49	J/mol×K	416.82	Joback Method
cpg	168.90	J/mol×K	445.89	Joback Method
cpg	176.93	J/mol×K	474.97	Joback Method
cpg	184.59	J/mol×K	504.04	Joback Method
dvisc	0.0052504	Pa×s	138.86	Joback Method
dvisc	0.0018368	Pa×s	170.65	Joback Method
dvisc	0.0008937	Pa×s	202.44	Joback Method
dvisc	0.0005287	Pa×s	234.23	Joback Method
dvisc	0.0003546	Pa×s	266.02	Joback Method
dvisc	0.0002590	Pa×s	297.81	Joback Method
dvisc	0.0002010	Pa×s	329.60	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38731e+01
Coeff. B	-2.63391e+03
Coeff. C	-4.46000e+01
Temperature range (K), min.	238.48
Temperature range (K), max.	352.24

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1115088&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/mol384.mol

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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