1,3-Pentadiene, 2-methyl-, (E)-

Other names:	(E)-1,3-Pentadiene, 2-methyl-
	(E)-CH2=C(CH3)CH=CHCH3
	2-Methyl-1,trans-3-pentadiene
	trans-2-Methyl-1,3-pentadiene
	trans-2-methylpenta-1,3-diene
Inchi:	InChI=1S/C6H10/c1-4-5-6(2)3/h4-5H,2H2,1,3H3/b5-4+
InchiKey:	RCJMVGJKROQDCB-SNAWJCMRSA-N
Formula:	C6H10
SMILES:	C=C(C)C=CC
Mol. weight [g/mol]:	82.14
CAS:	926-54-5

Physical Properties

Property code	Value	Unit	Source
gf	159.15	kJ/mol	Joback Method
hf	65.69	kJ/mol	Joback Method
hfus	8.91	kJ/mol	Joback Method
hvap	28.32	kJ/mol	Joback Method
ie	8.43	eV	NIST Webbook
ie	8.42 ± 0.03	eV	NIST Webbook
ie	8.47	eV	NIST Webbook
ie	8.45 ± 0.05	eV	NIST Webbook
ie	8.45	eV	NIST Webbook
log10ws	-2.04		Crippen Method
logp	2.139		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	627.30		NIST Webbook
rinpol	627.70		NIST Webbook
rinpol	627.00		NIST Webbook
tb	348.70	K	NIST Webbook
tb	348.85 ± 0.40	K	NIST Webbook
tc	517.19	K	Joback Method
tf	136.58	K	Joback Method
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.16	J/mol×K	337.40	Joback Method
cpg	142.08	J/mol×K	367.36	Joback Method
cpg	151.51	J/mol×K	397.33	Joback Method
cpg	160.47	J/mol×K	427.29	Joback Method
cpg	168.98	J/mol×K	457.26	Joback Method
cpg	177.07	J/mol×K	487.22	Joback Method
cpg	184.75	J/mol×K	517.19	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39713e+01
Coeff. B	-2.83619e+03
Coeff. C	-4.54610e+01
Temperature range (K), min.	252.73
Temperature range (K), max.	372.97

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C926545&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

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

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