1,3-PENTADIENE, 4-METHYL-

Other names:	(CH3)2C=CHCH=CH2
	4-methyl-1,3-pentadiene
	4-methylpenta-1,3-diene
Inchi:	InChI=1S/C6H10/c1-4-5-6(2)3/h4-5H,1H2,2-3H3
InchiKey:	CJSBUWDGPXGFGA-UHFFFAOYSA-N
Formula:	C6H10
SMILES:	C=CC=C(C)C
Mol. weight [g/mol]:	82.15
CAS:	926-56-7

Physical Properties

Property code	Value	Unit	Source
hf	56.98	kJ/mol	Cheméo Relay (1.0)
hfus	8.91	kJ/mol	Joback Method
hvap	30.09	kJ/mol	Cheméo Relay (1.0)
ie	8.26 ± 0.05	eV	NIST Webbook
ie	8.29	eV	NIST Webbook
ie	8.28 ± 0.02	eV	NIST Webbook
ie	8.25	eV	NIST Webbook
logp	2.139		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
rinpol	630.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	629.60		NIST Webbook
rinpol	628.70		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	609.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	636.00		NIST Webbook

ripol	777.00		NIST Webbook
ripol	746.00		NIST Webbook
ripol	796.00		NIST Webbook
tb	349.70	K	NIST Webbook
tb	347.00 ± 2.00	K	NIST Webbook
tb	349.00 ± 2.00	K	NIST Webbook
tb	349.45 ± 0.60	K	NIST Webbook
tb	350.00 ± 2.00	K	NIST Webbook
tf	203.00 ± 15.00	K	NIST Webbook

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	1.38441e+01
Coeff. B	-2.77744e+03
Coeff. C	-4.86470e+01
Temperature range (K), min.	253.53
Temperature range (K), max.	374.16

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0, beta):	
Cheméo Relay (1.0):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C926567&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol382.mol

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point