4-Methyl-1,3-pentadiene

Other names: (CH3)2C=CHCH=CH2
1,3-Pentadiene, 4-methyl-
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]: 82.14
CAS: 926-56-7

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	8.28 ± 0.02	eV	NIST Webbook
ie	8.26 ± 0.05	eV	NIST Webbook
ie	8.25	eV	NIST Webbook
ie	8.29	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	631.00		NIST Webbook
rinpol	629.60		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	628.00		NIST Webbook

rinpol	629.00		NIST Webbook
rinpol	628.70		NIST Webbook
rinpol	609.00		NIST Webbook
ripol	796.00		NIST Webbook
ripol	746.00		NIST Webbook
ripol	777.00		NIST Webbook
tb	349.70	K	NIST Webbook
tb	349.45 ± 0.60	K	NIST Webbook
tb	350.00 ± 2.00	K	NIST Webbook
tb	347.00 ± 2.00	K	NIST Webbook
tb	349.00 ± 2.00	K	NIST Webbook
tc	517.19	K	Joback Method
tf	203.00 ± 15.00	K	NIST Webbook
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	1.38441e+01
Coeff. B	-2.77744e+03
Coeff. C	-4.86470e+01
Temperature range (K), min.	253.53
Temperature range (K), max.	374.16

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol382.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C926567&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume