1,4-Pentadiene, 2-methyl-

Other names:	2-METHYL-4-PENTADIENE
	2-Methyl-1,4-pentadiene
	2-methylpenta-1,4-diene
Inchi:	InChI=1S/C6H10/c1-4-5-6(2)3/h4H,1-2,5H2,3H3
InchiKey:	DRWYRROCDFQZQF-UHFFFAOYSA-N
Formula:	C6H10
SMILES:	C=CCC(=C)C
Mol. weight [g/mol]:	82.14
CAS:	763-30-4

Physical Properties

Property code	Value	Unit	Source
gf	166.77	kJ/mol	Joback Method
hf	73.90	kJ/mol	Joback Method
hfus	7.43	kJ/mol	Joback Method
hvap	27.69	kJ/mol	Joback Method
ie	9.16 ± 0.05	eV	NIST Webbook
ie	9.16	eV	NIST Webbook
log10ws	-2.04		Crippen Method
logp	2.139		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	572.00		NIST Webbook
rinpol	580.00		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	578.00		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	578.00		NIST Webbook
rinpol	562.00		NIST Webbook
rinpol	580.00		NIST Webbook
tb	329.20	K	NIST Webbook
tb	331.00 ± 4.00	K	NIST Webbook
tc	503.72	K	Joback Method
tf	139.90	K	Joback Method
vc	0.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.15	J/mol×K	329.92	Joback Method
cpg	142.61	J/mol×K	358.89	Joback Method
cpg	151.66	J/mol×K	387.85	Joback Method
cpg	160.31	J/mol×K	416.82	Joback Method
cpg	168.57	J/mol×K	445.79	Joback Method
cpg	176.46	J/mol×K	474.76	Joback Method
cpg	184.00	J/mol×K	503.72	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.33360e+01
Coeff. B	-2.48932e+03
Coeff. C	-4.36500e+01
Temperature range (K), min.	234.43
Temperature range (K), max.	353.87

Sources

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/mol383.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C763304&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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