1,4-Hexadiene, 5-methyl-

Other names:	5-Methyl-1,4-hexadiene
	CH2=CHCH2CH=C(CH3)2
Inchi:	InChI=1S/C7H12/c1-4-5-6-7(2)3/h4,6H,1,5H2,2-3H3
InchiKey:	VSQLAQKFRFTMNS-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	C=CCC=C(C)C
Mol. weight [g/mol]:	96.17
CAS:	763-88-2

Physical Properties

Property code	Value	Unit	Source
gf	167.57	kJ/mol	Joback Method
hf	45.05	kJ/mol	Joback Method
hfus	11.50	kJ/mol	Joback Method
hvap	30.54	kJ/mol	Joback Method
ie	8.70	eV	NIST Webbook
log10ws	-2.46		Crippen Method
logp	2.529		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
tb	364.90 ± 2.00	K	NIST Webbook
tb	365.00 ± 2.00	K	NIST Webbook
tc	539.87	K	Joback Method
tf	147.85	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.59	J/mol×K	360.28	Joback Method
cpg	177.90	J/mol×K	390.21	Joback Method
cpg	188.66	J/mol×K	420.14	Joback Method
cpg	198.89	J/mol×K	450.07	Joback Method
cpg	208.63	J/mol×K	480.01	Joback Method

cpg	217.89	J/mol×K	509.94	Joback Method
cpg	226.70	J/mol×K	539.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C763882&Units=SI
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

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