1,5-Hexadiene, 3-methyl-

Other names: 3-Methyl-1,5-hexadiene
Inchi: InChI=1S/C7H12/c1-4-6-7(3)5-2/h4-5,7H,1-2,6H2,3H3
InchiKey: JXENLILXUMZMFC-UHFFFAOYSA-N
Formula: C7H12
SMILES: C=CCC(C)C=C
Mol. weight [g/mol]: 96.17
CAS: 1541-33-9

Physical Properties

Property code	Value	Unit	Source
gf	181.30	kJ/mol	Joback Method
hf	57.77	kJ/mol	Joback Method
hfus	7.80	kJ/mol	Joback Method
hvap	29.45	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.385		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	637.00		NIST Webbook
rinpol	633.00		NIST Webbook
rinpol	637.00		NIST Webbook
tb	353.15 ± 0.50	K	NIST Webbook
tb	354.00 ± 2.00	K	NIST Webbook
tb	353.70 ± 2.00	K	NIST Webbook
tb	353.20	K	NIST Webbook
tc	527.02	K	Joback Method
tf	150.13	K	Joback Method
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.80	J/mol×K	352.48	Joback Method
cpg	177.85	J/mol×K	381.57	Joback Method

cpg	188.42	J/mol×K	410.66	Joback Method
cpg	198.52	J/mol×K	439.75	Joback Method
cpg	208.17	J/mol×K	468.84	Joback Method
cpg	217.38	J/mol×K	497.93	Joback Method
cpg	226.18	J/mol×K	527.02	Joback Method
dvisc	0.0061775	Pa×s	150.13	Joback Method
dvisc	0.0021155	Pa×s	183.85	Joback Method
dvisc	0.0010099	Pa×s	217.58	Joback Method
dvisc	0.0005880	Pa×s	251.31	Joback Method
dvisc	0.0003891	Pa×s	285.03	Joback Method
dvisc	0.0002810	Pa×s	318.75	Joback Method
dvisc	0.0002159	Pa×s	352.48	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=392
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1541339&Units=SI
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
dvisc:	Dynamic viscosity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume