

1,5-Hexadiene, 3,4-dimethyl-

Inchi:	InChI=1S/C8H14/c1-5-7(3)8(4)6-2/h5-8H,1-2H2,3-4H3
InchiKey:	BKVALJGAKNDDJJ-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	C=CC(C)C(C)C=C
Mol. weight [g/mol]:	110.20
CAS:	4894-63-7

Physical Properties

Property code	Value	Unit	Source
gf	187.28	kJ/mol	Joback Method
hf	31.85	kJ/mol	Joback Method
hfus	6.87	kJ/mol	Joback Method
hvap	31.29	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.631		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
tb	374.95 ± 0.50	K	NIST Webbook
tc	553.30	K	Joback Method
tf	146.40	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.12	J/mol×K	374.92	Joback Method
cpg	215.84	J/mol×K	404.65	Joback Method
cpg	228.00	J/mol×K	434.38	Joback Method
cpg	239.61	J/mol×K	464.11	Joback Method
cpg	250.68	J/mol×K	493.84	Joback Method
cpg	261.25	J/mol×K	523.57	Joback Method
cpg	271.33	J/mol×K	553.30	Joback Method
dvisc	0.0145037	Pa×s	146.40	Joback Method
dvisc	0.0034956	Pa×s	184.49	Joback Method

dvisc	0.0013710	Pa×s	222.57	Joback Method
dvisc	0.0007069	Pa×s	260.66	Joback Method
dvisc	0.0004316	Pa×s	298.75	Joback Method
dvisc	0.0002946	Pa×s	336.83	Joback Method
dvisc	0.0002173	Pa×s	374.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4894637&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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