

4-Methyl-1,5-Heptadiene

Inchi:	InChI=1S/C8H14/c1-4-6-8(3)7-5-2/h4-5,7-8H,1,6H2,2-3H3/b7-5+
InchiKey:	ITKKJSFRRSLPHX-FNORWQNLSA-N
Formula:	C8H14
SMILES:	C=CCC(C)C=CC
Mol. weight [g/mol]:	110.20
CAS:	998-94-7

Physical Properties

Property code	Value	Unit	Source
gf	182.10	kJ/mol	Joback Method
hf	28.92	kJ/mol	Joback Method
hfus	11.88	kJ/mol	Joback Method
hvap	32.30	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.775		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
tb	383.50 ± 1.00	K	NIST Webbook
tb	400.00 ± 1.00	K	NIST Webbook
tc	562.47	K	Joback Method
tf	158.08	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.36	J/mol×K	382.84	Joback Method
cpg	261.23	J/mol×K	532.53	Joback Method
cpg	250.77	J/mol×K	502.59	Joback Method
cpg	239.78	J/mol×K	472.65	Joback Method
cpg	228.23	J/mol×K	442.72	Joback Method
cpg	216.10	J/mol×K	412.78	Joback Method
cpg	271.18	J/mol×K	562.47	Joback Method
dvisc	0.0001898	Pa×s	382.84	Joback Method

dvisc	0.0002528	Pa×s	345.38	Joback Method
dvisc	0.0003612	Pa×s	307.92	Joback Method
dvisc	0.0005696	Pa×s	270.46	Joback Method
dvisc	0.0010398	Pa×s	233.00	Joback Method
dvisc	0.0023908	Pa×s	195.54	Joback Method
dvisc	0.0081563	Pa×s	158.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C998947&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccol:	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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