1,5-Heptadiene, 3-methyl-

Other names: 3-Methyl-1,5-heptadiene
Inchi: InChI=1S/C8H14/c1-4-6-7-8(3)5-2/h4-6,8H,2,7H2,1,3H3/b6-4+
InchiKey: QIWJMWAOAINRPL-GQCTYLIASA-N
Formula: C8H14
SMILES: C=CC(C)CC=CC
Mol. weight [g/mol]: 110.20
CAS: 4894-62-6

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	383.70 ± 1.00	K	NIST Webbook
tb	385.70 ± 2.00	K	NIST Webbook
tb	384.15 ± 0.50	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	216.10	J/mol×K	412.78	Joback Method
cpg	228.23	J/mol×K	442.72	Joback Method
cpg	239.78	J/mol×K	472.65	Joback Method
cpg	250.77	J/mol×K	502.59	Joback Method
cpg	261.23	J/mol×K	532.53	Joback Method

cpg	271.18	J/mol×K	562.47	Joback Method
dvisc	0.0081563	Pa×s	158.08	Joback Method
dvisc	0.0023908	Pa×s	195.54	Joback Method
dvisc	0.0010398	Pa×s	233.00	Joback Method
dvisc	0.0005696	Pa×s	270.46	Joback Method
dvisc	0.0003612	Pa×s	307.92	Joback Method
dvisc	0.0002528	Pa×s	345.38	Joback Method
dvisc	0.0001898	Pa×s	382.84	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56130e+01
Coeff. B	-3.69152e+03
Coeff. C	-4.79440e+01
Temperature range (K), min.	288.82
Temperature range (K), max.	406.29

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4894626&Units=SI

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