1,4-Heptadiene, 3-methyl-

Other names: 3-Methyl-1,4-heptadiene
Inchi: InChI=1S/C8H14/c1-4-6-7-8(3)5-2/h5-8H,2,4H2,1,3H3/b7-6+
InchiKey: FBJNXQPYIFUANI-VOTSOKGWSA-N
Formula: C8H14
SMILES: C=CC(C)C=CCC
Mol. weight [g/mol]: 110.20
CAS: 1603-01-6

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
rinpol	715.00		NIST Webbook
rinpol	715.00		NIST Webbook
tb	378.10 ± 0.40	K	NIST Webbook
tb	378.40 ± 0.60	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

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1603016&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
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