1,4-Hexadiene, 3-ethyl-

Other names: 3-Ethyl-1,4-hexadiene
Inchi: InChI=1S/C8H14/c1-4-7-8(5-2)6-3/h4-5,7-8H,2,6H2,1,3H3/b7-4+
InchiKey: AGZNHDUBGPTFIN-QPJJXVBHSA-N
Formula: C8H14
SMILES: C=CC(C=CC)CC
Mol. weight [g/mol]: 110.20
CAS: 2080-89-9

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	903.00		NIST Webbook
rinpol	903.00		NIST Webbook
tb	382.84	K	Joback Method
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

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=C2080899&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

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