2,4-Hexadiene, (E,Z)-

Other names:	(E),(Z)-CH3CH=CHCH=CHCH3
	(E,Z)-2,4-HEXADIENE
	(Z,E)-2,4-Hexadiene
	CIS,TRANS-2,4-HEXADIENE
	cis,trans-hexa-2,4-diene
Inchi:	InChI=1S/C6H10/c1-3-5-6-4-2/h3-6H,1-2H3/b5-3-,6-4+
InchiKey:	APPOKADJQUIAHP-CIIODKQPSA-N
Formula:	C6H10
SMILES:	CC=CC=CC
Mol. weight [g/mol]:	82.14
CAS:	5194-50-3

Physical Properties

Property code	Value	Unit	Source
gf	160.08	kJ/mol	Joback Method
hf	48.00 ± 2.00	kJ/mol	NIST Webbook
hfus	11.70	kJ/mol	Joback Method
hvap	28.87	kJ/mol	Joback Method
ie	8.25 ± 0.02	eV	NIST Webbook
ie	8.24 ± 0.05	eV	NIST Webbook
ie	8.26	eV	NIST Webbook
ie	8.22	eV	NIST Webbook
log10ws	-2.04		Crippen Method
logp	2.139		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpol	636.40		NIST Webbook
rinpol	673.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	673.00		NIST Webbook
rinpol	653.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	656.00		NIST Webbook
tb	354.20	K	NIST Webbook
tb	356.62 ± 0.40	K	NIST Webbook
tc	527.01	K	Joback Method

tf	177.10 ± 0.40	K	NIST Webbook
vc	0.332	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	131.24	J/mol×K	345.00	Joback Method
cpg	176.95	J/mol×K	496.67	Joback Method
cpg	168.79	J/mol×K	466.34	Joback Method
cpg	160.17	J/mol×K	436.00	Joback Method
cpg	151.05	J/mol×K	405.67	Joback Method
cpg	141.42	J/mol×K	375.33	Joback Method
cpg	184.66	J/mol×K	527.01	Joback Method
dvisc	0.0001508	Pa×s	345.00	Joback Method
dvisc	0.0001943	Pa×s	312.04	Joback Method
dvisc	0.0002657	Pa×s	279.07	Joback Method
dvisc	0.0003954	Pa×s	246.11	Joback Method
dvisc	0.0006652	Pa×s	213.15	Joback Method
dvisc	0.0013538	Pa×s	180.18	Joback Method
dvisc	0.0037874	Pa×s	147.22	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.03125e+01
Coeff. B	-5.90969e+03
Coeff. C	-6.75131e+00
Coeff. D	4.22754e-06
Temperature range (K), min.	177.05
Temperature range (K), max.	538.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=374
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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=374
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5194503&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume