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

Other names:	(2Z,4Z)-2,4-Hexadiene
	(Z),(Z)-CH3CH=CHCH=CHCH3
	(Z,Z)-2,4-HEXADIENE
	2,4-Hexadiene, (Z,Z)-
	CIS,CIS-2,4-HEXADIENE
	cis-2,cis-4-Hexadiene
Inchi:	InChI=1S/C6H10/c1-3-5-6-4-2/h3-6H,1-2H3/b5-3-,6-4-
InchiKey:	APPOKADJQUIAHP-GLIMQPGKSA-N
Formula:	C6H10
SMILES:	CC=CC=CC
Mol. weight [g/mol]:	82.14
CAS:	6108-61-8

Physical Properties

Property code	Value	Unit	Source
gf	160.08	kJ/mol	Joback Method
hf	52.00 ± 2.00	kJ/mol	NIST Webbook
hfus	11.70	kJ/mol	Joback Method
hvap	28.87	kJ/mol	Joback Method
ie	8.18 ± 0.02	eV	NIST Webbook
ie	8.27	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	661.30		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	660.40		NIST Webbook
rinpol	661.00		NIST Webbook
tb	358.08 ± 0.20	K	NIST Webbook
tc	527.01	K	Joback Method
tf	203.78 ± 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	141.42	J/mol×K	375.33	Joback Method
cpg	151.05	J/mol×K	405.67	Joback Method
cpg	160.17	J/mol×K	436.00	Joback Method
cpg	168.79	J/mol×K	466.34	Joback Method
cpg	176.95	J/mol×K	496.67	Joback Method
cpg	184.66	J/mol×K	527.01	Joback Method
dvisc	0.0037874	Pa×s	147.22	Joback Method
dvisc	0.0013538	Pa×s	180.18	Joback Method
dvisc	0.0006652	Pa×s	213.15	Joback Method
dvisc	0.0003954	Pa×s	246.11	Joback Method
dvisc	0.0002657	Pa×s	279.07	Joback Method
dvisc	0.0001943	Pa×s	312.04	Joback Method
dvisc	0.0001508	Pa×s	345.00	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34840e+01
Coeff. B	-2.73711e+03
Coeff. C	-4.93500e+01
Temperature range (K), min.	256.76
Temperature range (K), max.	384.26

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6108618&Units=SI

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

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=373
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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