(E)-1,3-Hexadiene

Other names: 1,3-Hexadiene, (E)-
1,trans-3-hexadiene
Inchi: InChI=1S/C6H10/c1-3-5-6-4-2/h3,5-6H,1,4H2,2H3/b6-5+
InchiKey: AHAREKHAZNPPMI-AATRIKPKSA-N
Formula: C6H10
SMILES: C=CC=CCC
Mol. weight [g/mol]: 82.14
CAS: 20237-34-7

Physical Properties

Property code	Value	Unit	Source
gf	167.70	kJ/mol	Joback Method
hf	54.00 ± 2.00	kJ/mol	NIST Webbook
hfus	10.22	kJ/mol	Joback Method
hvap	28.24	kJ/mol	Joback Method
ie	8.51	eV	NIST Webbook
ie	8.53 ± 0.02	eV	NIST Webbook
ie	8.54 ± 0.05	eV	NIST Webbook
log10ws	-2.04		Crippen Method
logp	2.139		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
rinpol	614.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	612.50		NIST Webbook
rinpol	612.00		NIST Webbook
tb	346.40 ± 0.60	K	NIST Webbook
tc	513.57	K	Joback Method
tf	170.80 ± 0.60	K	NIST Webbook
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.12	J/mol×K	337.52	Joback Method
cpg	176.34	J/mol×K	484.23	Joback Method
cpg	168.36	J/mol×K	454.89	Joback Method
cpg	159.96	J/mol×K	425.54	Joback Method
cpg	151.13	J/mol×K	396.20	Joback Method
cpg	141.86	J/mol×K	366.86	Joback Method
cpg	183.93	J/mol×K	513.57	Joback Method
dvisc	0.0001758	Pa×s	337.52	Joback Method
dvisc	0.0002228	Pa×s	306.36	Joback Method
dvisc	0.0002980	Pa×s	275.19	Joback Method
dvisc	0.0004292	Pa×s	244.03	Joback Method
dvisc	0.0006879	Pa×s	212.87	Joback Method
dvisc	0.0012964	Pa×s	181.70	Joback Method
dvisc	0.0031761	Pa×s	150.54	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36864e+01
Coeff. B	-2.58152e+03
Coeff. C	-6.17180e+01
Temperature range (K), min.	254.39
Temperature range (K), max.	369.96

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20237347&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
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