1,3,5-Hexatriene

Other names:	Divinylethylene
	Hexa-1,3,5-triene
	Hexatriene
	hexa-1,3,5-triene, mixed isomers
Inchi:	InChI=1S/C6H8/c1-3-5-6-4-2/h3-6H,1-2H2
InchiKey:	AFVDZBIIBXWASR-UHFFFAOYSA-N
Formula:	C6H8
SMILES:	C=CC=CC=C
Mol. weight [g/mol]:	80.13
CAS:	2235-12-3

Physical Properties

Property code	Value	Unit	Source
gf	255.54	kJ/mol	Joback Method
hf	200.91	kJ/mol	Joback Method
hfus	8.94	kJ/mol	Joback Method
hvap	27.57	kJ/mol	Joback Method
ie	8.42 ± 0.05	eV	NIST Webbook
ie	8.27 ± 0.05	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	1.915		Crippen Method
mcvol	82.500	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
rinpol	648.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	648.00		NIST Webbook
tb	334.20	K	Joback Method
tc	514.08	K	Joback Method
tf	261.45 ± 0.30	K	NIST Webbook
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	119.39	J/mol×K	334.20	Joback Method
cpg	128.51	J/mol×K	364.18	Joback Method
cpg	137.13	J/mol×K	394.16	Joback Method
cpg	145.27	J/mol×K	424.14	Joback Method
cpg	152.97	J/mol×K	454.12	Joback Method
cpg	160.23	J/mol×K	484.10	Joback Method
cpg	167.09	J/mol×K	514.08	Joback Method
dvisc	0.0024391	Pa×s	148.78	Joback Method
dvisc	0.0010595	Pa×s	179.68	Joback Method
dvisc	0.0005878	Pa×s	210.59	Joback Method
dvisc	0.0003792	Pa×s	241.49	Joback Method
dvisc	0.0002702	Pa×s	272.39	Joback Method
dvisc	0.0002063	Pa×s	303.30	Joback Method
dvisc	0.0001656	Pa×s	334.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49077e+01
Coeff. B	-3.22923e+03
Coeff. C	-3.91590e+01
Temperature range (K), min.	260.03
Temperature range (K), max.	375.67

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2235123&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

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