1,3,5-Heptatriene, (E,E)-

Other names:	All-trans-1,3,5-Heptatriene
	(E,E)-CH2=CHCH=CHCH=CHCH3
	trans,trans-1,3,5-Heptatriene
	(3E,5E)-1,3,5-Heptatriene
	(E,E)-1,3,5-heptatriene
Inchi:	InChI=1S/C7H10/c1-3-5-7-6-4-2/h3-7H,1H2,2H3/b6-4+,7-5+
InchiKey:	USKZHEQYENVSMH-YDFGWWAZSA-N
Formula:	C7H10
SMILES:	C=CC=CC=CC
Mol. weight [g/mol]:	94.15
CAS:	17679-93-5

Physical Properties

Property code	Value	Unit	Source
gf	256.34	kJ/mol	Joback Method
hf	172.06	kJ/mol	Joback Method
hfus	13.01	kJ/mol	Joback Method
hvap	30.42	kJ/mol	Joback Method
ie	8.07	eV	NIST Webbook
ie	7.96 ± 0.02	eV	NIST Webbook
log10ws	-2.31		Crippen Method
logp	2.305		Crippen Method
mcvol	96.590	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	781.00		NIST Webbook
ripol	1005.00		NIST Webbook
tb	364.56	K	Joback Method
tc	550.14	K	Joback Method
tf	156.73	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	152.45	J/mol×K	364.56	Joback Method
cpg	201.01	J/mol×K	519.21	Joback Method
cpg	192.43	J/mol×K	488.28	Joback Method
cpg	183.31	J/mol×K	457.35	Joback Method
cpg	173.63	J/mol×K	426.42	Joback Method
cpg	163.36	J/mol×K	395.49	Joback Method
cpg	209.10	J/mol×K	550.14	Joback Method
dvisc	0.0001546	Pa×s	364.56	Joback Method
dvisc	0.0001979	Pa×s	329.92	Joback Method
dvisc	0.0002684	Pa×s	295.28	Joback Method
dvisc	0.0003947	Pa×s	260.64	Joback Method
dvisc	0.0006532	Pa×s	226.01	Joback Method
dvisc	0.0012974	Pa×s	191.37	Joback Method
dvisc	0.0034902	Pa×s	156.73	Joback Method

Sources

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=C17679935&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
ripol: Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume