1,5-Heptadiene, (E)-

Other names:	trans-1,5-Heptadiene
	1,5-Heptadiene
	(5E)-1,5-Heptadiene
	1,trans-5-Heptadiene
Inchi:	InChI=1S/C7H12/c1-3-5-7-6-4-2/h3-4,6H,1,5,7H2,2H3/b6-4+
InchiKey:	ZGXMNEKDFYUNDQ-GQCTYLIASA-N
Formula:	C7H12
SMILES:	C=CCCC=CC
Mol. weight [g/mol]:	96.17
CAS:	7736-22-3

Physical Properties

Property code	Value	Unit	Source
gf	176.12	kJ/mol	Joback Method
hf	54.84	kJ/mol	Joback Method
hfus	12.81	kJ/mol	Joback Method
hvap	30.46	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.529		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	678.80		NIST Webbook
rinpol	682.00		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	681.90		NIST Webbook
tb	360.40	K	Joback Method
tc	536.35	K	Joback Method
tf	161.81	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.57	J/mol×K	360.40	Joback Method

cpg	177.68	J/mol×K	389.72	Joback Method
cpg	188.27	J/mol×K	419.05	Joback Method
cpg	198.35	J/mol×K	448.37	Joback Method
cpg	207.96	J/mol×K	477.70	Joback Method
cpg	217.10	J/mol×K	507.02	Joback Method
cpg	225.80	J/mol×K	536.35	Joback Method
dvisc	0.0037899	Pa×s	161.81	Joback Method
dvisc	0.0015040	Pa×s	194.91	Joback Method
dvisc	0.0007806	Pa×s	228.01	Joback Method
dvisc	0.0004784	Pa×s	261.11	Joback Method
dvisc	0.0003273	Pa×s	294.20	Joback Method
dvisc	0.0002418	Pa×s	327.30	Joback Method
dvisc	0.0001889	Pa×s	360.40	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7736223&Units=SI
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

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

vc: Critical Volume