1,5-Heptadiene

Other names: Hepta-1,5-diene
Inchi: InChI=1S/C7H12/c1-3-5-7-6-4-2/h3-4,6H,1,5,7H2,2H3
InchiKey: ZGXMNEKDFYUNDQ-UHFFFAOYSA-N
Formula: C7H12
SMILES: C=CCCC=CC
Mol. weight [g/mol]: 96.17
CAS: 1541-23-7

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	691.60		NIST Webbook
rinpol	696.80		NIST Webbook
rinpol	695.30		NIST Webbook
rinpol	691.00		NIST Webbook
tb	367.40 ± 1.00	K	NIST Webbook
tb	366.85 ± 0.50	K	NIST Webbook
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	217.10	J/mol×K	507.02	Joback Method
cpg	207.96	J/mol×K	477.70	Joback Method

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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55181e+01
Coeff. B	-3.53351e+03
Coeff. C	-4.32180e+01
Temperature range (K), min.	275.22
Temperature range (K), max.	389.42

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1541237&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
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