1,4-Heptadiene

Inchi: InChI=1S/C7H12/c1-3-5-7-6-4-2/h3,6-7H,1,4-5H2,2H3
InchiKey: FMAMSYPJXSEYSW-UHFFFAOYSA-N
Formula: C7H12
SMILES: C=CCC=CCC
Mol. weight [g/mol]: 96.17
CAS: 5675-22-9

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
tb	366.23 ± 0.60	K	NIST Webbook
tb	373.90 ± 5.00	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	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55469e+01
Coeff. B	-3.53223e+03
Coeff. C	-4.29400e+01
Temperature range (K), min.	274.42
Temperature range (K), max.	388.04

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=C5675229&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

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