3-Heptene

Other names: 3-Heptene (c,t)
hept-3-ene
Inchi: InChI=1S/C7H14/c1-3-5-7-6-4-2/h5,7H,3-4,6H2,1-2H3
InchiKey: WZHKDGJSXCTSCK-UHFFFAOYSA-N
Formula: C7H14
SMILES: CCC=CCCC
Mol. weight [g/mol]: 98.19
CAS: 592-78-9

Physical Properties

Property code	Value	Unit	Source
chl	-4646.88 ± 0.71	kJ/mol	NIST Webbook
gf	88.28	kJ/mol	Joback Method
hf	-70.59	kJ/mol	Joback Method
hfus	14.09	kJ/mol	Joback Method
hvap	31.13	kJ/mol	Joback Method
ie	8.77 ± 0.02	eV	NIST Webbook
log10ws	-2.61		Crippen Method
logp	2.753		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
rinpol	698.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	708.30		NIST Webbook
tb	368.65 ± 2.00	K	NIST Webbook
tb	367.15 ± 2.00	K	NIST Webbook
tb	367.15 ± 2.00	K	NIST Webbook
tb	368.80 ± 2.00	K	NIST Webbook
tb	367.15 ± 2.00	K	NIST Webbook
tb	368.90 ± 1.00	K	NIST Webbook
tb	368.90 ± 1.00	K	NIST Webbook
tb	368.70 ± 1.00	K	NIST Webbook
tb	367.15 ± 2.00	K	NIST Webbook
tb	369.05 ± 1.00	K	NIST Webbook
tb	369.65 ± 2.00	K	NIST Webbook

tb	369.00 ± 1.00	K	NIST Webbook
tb	368.75 ± 0.70	K	NIST Webbook
tb	368.90 ± 0.50	K	NIST Webbook
tb	368.95 ± 1.00	K	NIST Webbook
tb	368.65 ± 2.00	K	NIST Webbook
tb	369.20 ± 1.00	K	NIST Webbook
tb	369.20 ± 1.00	K	NIST Webbook
tb	369.25 ± 1.00	K	NIST Webbook
tb	370.65 ± 2.00	K	NIST Webbook
tc	536.01	K	Joback Method
tf	163.57	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.32	J/mol×K	363.72	Joback Method
cpg	233.95	J/mol×K	507.29	Joback Method
cpg	224.15	J/mol×K	478.58	Joback Method
cpg	213.90	J/mol×K	449.86	Joback Method
cpg	203.19	J/mol×K	421.15	Joback Method
cpg	192.00	J/mol×K	392.43	Joback Method
cpg	243.33	J/mol×K	536.01	Joback Method
dvisc	0.0001967	Pa×s	363.72	Joback Method
dvisc	0.0002558	Pa×s	330.36	Joback Method
dvisc	0.0003528	Pa×s	297.00	Joback Method
dvisc	0.0005278	Pa×s	263.64	Joback Method
dvisc	0.0008875	Pa×s	230.29	Joback Method
dvisc	0.0017796	Pa×s	196.93	Joback Method
dvisc	0.0047393	Pa×s	163.57	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49153e+01
Coeff. B	-3.34928e+03

Coeff. C	-4.37320e+01
Temperature range (K), min.	272.70
Temperature range (K), max.	392.48

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=C592789&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
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