2-Heptene

Other names: 2-C7H14
Hept-2-ene
Heptene-2
Inchi: InChI=1S/C7H14/c1-3-5-7-6-4-2/h3,5H,4,6-7H2,1-2H3
InchiKey: OTTZHAVKAVGASB-UHFFFAOYSA-N
Formula: C7H14
SMILES: CC=CCCCC
Mol. weight [g/mol]: 98.19
CAS: 592-77-8

Physical Properties

Property code	Value	Unit	Source
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	8.84 ± 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	703.00		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	729.00		NIST Webbook
tb	371.40 ± 0.80	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	192.00	J/mol×K	392.43	Joback Method
cpg	203.19	J/mol×K	421.15	Joback Method
cpg	213.90	J/mol×K	449.86	Joback Method
cpg	224.15	J/mol×K	478.58	Joback Method
cpg	233.95	J/mol×K	507.29	Joback Method
cpg	243.33	J/mol×K	536.01	Joback Method
dvisc	0.0047393	Pa×s	163.57	Joback Method
dvisc	0.0017796	Pa×s	196.93	Joback Method
dvisc	0.0008875	Pa×s	230.29	Joback Method
dvisc	0.0005278	Pa×s	263.64	Joback Method
dvisc	0.0003528	Pa×s	297.00	Joback Method
dvisc	0.0002558	Pa×s	330.36	Joback Method
dvisc	0.0001967	Pa×s	363.72	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49203e+01
Coeff. B	-3.36875e+03
Coeff. C	-4.43990e+01
Temperature range (K), min.	274.62
Temperature range (K), max.	394.99

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C592778&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

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume