4-Hexen-3-ol

Other names:	2-Hexen-4-ol
	Allyl alcohol, 1-ethyl-3-methyl-
	hex-4-en-3-ol
	«alpha»-Ethyl-«gamma»-methylallyl alcohol
	Â«alphaÂ»-Ethyl-Â«gammaÂ»-methylallyl alcohol
Inchi:	InChI=1S/C6H12O/c1-3-5-6(7)4-2/h3,5-7H,4H2,1-2H3/b5-3+
InchiKey:	KWUXUOPPQQMMIL-HWKANZROSA-N
Formula:	C6H12O
SMILES:	CC=CC(O)CC
Mol. weight [g/mol]:	100.16
CAS:	4798-58-7

Physical Properties

Property code	Value	Unit	Source
gf	-59.40	kJ/mol	Joback Method
hf	-207.46	kJ/mol	Joback Method
hfus	12.06	kJ/mol	Joback Method
hvap	45.20	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.333		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
tb	408.40 ± 1.50	K	NIST Webbook
tc	605.02	K	Joback Method
tf	198.12	K	Joback Method
vc	0.364	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.87	J/mol×K	432.58	Joback Method
cpg	234.96	J/mol×K	576.28	Joback Method
cpg	227.13	J/mol×K	547.54	Joback Method
cpg	218.92	J/mol×K	518.80	Joback Method

cpg	210.32	J/mol×K	490.06	Joback Method
cpg	201.31	J/mol×K	461.32	Joback Method
cpg	242.44	J/mol×K	605.02	Joback Method
dvisc	0.0001926	Pa×s	432.58	Joback Method
dvisc	0.0003506	Pa×s	393.50	Joback Method
dvisc	0.0007282	Pa×s	354.43	Joback Method
dvisc	0.0018131	Pa×s	315.35	Joback Method
dvisc	0.0058431	Pa×s	276.27	Joback Method
dvisc	0.0276896	Pa×s	237.20	Joback Method
dvisc	0.2423961	Pa×s	198.12	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59699e+01
Coeff. B	-4.01521e+03
Coeff. C	-5.46850e+01
Temperature range (K), min.	310.72
Temperature range (K), max.	431.40

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4798587&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume