3-Hexen-1-ol, (E)-

Other names:	(3E)-Hexenol
	(E)-3-Hexen-1-ol
	(E)-Hex-3-en-1-ol
	(E)-Hex-3-enol
	3(E)-hexen-1-ol
	E-3-Hexenol
	trans-3-Hexen-1-ol
	trans-3-Hexenol
	trans-Hex-3-en-1-ol
Inchi:	InChI=1S/C6H12O/c1-2-3-4-5-6-7/h3-4,7H,2,5-6H2,1H3/b4-3+
InchiKey:	UFLHIIWVXFIJGU-ONEGZZNKSA-N
Formula:	C6H12O
SMILES:	CCC=CCCO
Mol. weight [g/mol]:	100.16
CAS:	928-97-2

Physical Properties

Property code	Value	Unit	Source
gf	-56.96	kJ/mol	Joback Method
hf	-202.18	kJ/mol	Joback Method
hfus	15.59	kJ/mol	Joback Method
hvap	45.59	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	1.335		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
rinpol	824.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	858.00		NIST Webbook
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ripol	1366.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1326.00		NIST Webbook
ripol	1351.00		NIST Webbook
tb	427.70	K	NIST Webbook
tc	601.76	K	Joback Method
tf	213.12	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.78	J/mol×K	433.02	Joback Method
cpg	200.94	J/mol×K	461.14	Joback Method
cpg	209.69	J/mol×K	489.27	Joback Method
cpg	218.06	J/mol×K	517.39	Joback Method
cpg	226.05	J/mol×K	545.51	Joback Method
cpg	233.69	J/mol×K	573.64	Joback Method

cpg	240.99	J/mol×K	601.76	Joback Method
dvisc	0.0918576	Pa×s	213.12	Joback Method
dvisc	0.0156415	Pa×s	249.77	Joback Method
dvisc	0.0041899	Pa×s	286.42	Joback Method
dvisc	0.0015133	Pa×s	323.07	Joback Method
dvisc	0.0006726	Pa×s	359.72	Joback Method
dvisc	0.0003473	Pa×s	396.37	Joback Method
dvisc	0.0002006	Pa×s	433.02	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	334.70	K	1.60	NIST Webbook
tbrp	334.50 ± 0.50	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61892e+01
Coeff. B	-4.24776e+03
Coeff. C	-6.05930e+01
Temperature range (K), min.	327.72
Temperature range (K), max.	451.09

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=C928972&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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