

(Z)-3-Hexen-1-ol

Other names:	cis-3-hexen-1-ol cis-3-hexenol
Inchi:	InChI=1S/C6H12O/c1-2-3-4-5-6-7/h3-4,7H,2,5-6H2,1H3/b4-3-
InchiKey:	UFLHIIWVXFJGU-ARJAWSKDSA-N
Formula:	C6H12O
SMILES:	CCC=CCCO
Mol. weight [g/mol]:	100.16

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
ripol	836.00		NIST Webbook
ripol	849.00		NIST Webbook
ripol	858.00		NIST Webbook
ripol	852.00		NIST Webbook
ripol	849.00		NIST Webbook
ripol	833.00		NIST Webbook
ripol	1389.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1379.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1395.00		NIST Webbook
ripol	1394.00		NIST Webbook
ripol	1379.00		NIST Webbook
ripol	1393.00		NIST Webbook
tb	433.02	K	Joback Method
tc	601.76	K	Joback Method

tf	213.12	K	Joback Method
vc	0.370	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.69	J/molxK	489.27	Joback Method
cpg	240.99	J/molxK	601.76	Joback Method
cpg	233.69	J/molxK	573.64	Joback Method
cpg	226.05	J/molxK	545.51	Joback Method
cpg	218.06	J/molxK	517.39	Joback Method
cpg	191.78	J/molxK	433.02	Joback Method
cpg	200.94	J/molxK	461.14	Joback Method
dvisc	0.0041899	Paxs	286.42	Joback Method
dvisc	0.0015133	Paxs	323.07	Joback Method
dvisc	0.0003473	Paxs	396.37	Joback Method
dvisc	0.0002006	Paxs	433.02	Joback Method
dvisc	0.0006726	Paxs	359.72	Joback Method
dvisc	0.0918576	Paxs	213.12	Joback Method
dvisc	0.0156415	Paxs	249.77	Joback Method
pvap	3.39e-03	kPa	258.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.21	kPa	303.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.21	kPa	303.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol

pvap	0.21	kPa	303.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.30	kPa	308.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	3.01e-04	kPa	238.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	3.03e-04	kPa	238.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	3.04e-04	kPa	238.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	5.77e-04	kPa	243.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	5.79e-04	kPa	243.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol

pvap	5.80e-04	kPa	243.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	1.06e-03	kPa	248.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	1.07e-03	kPa	248.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	1.07e-03	kPa	248.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	1.92e-03	kPa	253.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	1.92e-03	kPa	253.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	1.93e-03	kPa	253.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol

pvap	3.38e-03	kPa	258.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.30	kPa	308.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	3.40e-03	kPa	258.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	5.80e-03	kPa	263.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	5.80e-03	kPa	263.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	5.81e-03	kPa	263.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	9.73e-03	kPa	268.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol

pvap	9.73e-03	kPa	268.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	9.74e-03	kPa	268.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.02	kPa	273.65	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.02	kPa	273.65	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.02	kPa	273.65	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.03	kPa	278.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.03	kPa	278.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol

pvap	0.03	kPa	278.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.04	kPa	283.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.04	kPa	283.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.04	kPa	283.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.06	kPa	288.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.06	kPa	288.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.06	kPa	288.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol

pvap	0.09	kPa	293.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.09	kPa	293.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.09	kPa	293.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.14	kPa	298.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.14	kPa	298.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.14	kPa	298.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.30	kPa	308.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol

rho_l	833.27	kg/m ³	318.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution
rho_l	840.99	kg/m ³	308.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution
rho_l	848.64	kg/m ³	298.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution
rho_l	852.44	kg/m ³	293.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution
rho_l	856.22	kg/m ³	288.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor pressures and thermophysical properties of selected hexenols and their homologs	https://www.doi.org/10.1016/j.fluid.2015.05.026
Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution	https://www.doi.org/10.1021/je300280s
Flow Aqueous Volatiles on Atmospheric Air/Water Interfaces: A Combined Experimental and Molecular Simulation Study	https://www.doi.org/10.1021/je500114m
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=R599452&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
rho:	Liquid Density
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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