1-Hexen-3-ol

Other names:	1-Hexene-3-ol
	3-Hydroxy-1-hexene
	Hex-1-en-3-ol
	Hexen-3-ol
	Propylvinylcarbinol
Inchi:	InChI=1S/C6H12O/c1-3-5-6(7)4-2/h4,6-7H,2-3,5H2,1H3
InchiKey:	BVOSSZSHBZQJOI-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	C=CC(O)CCC
Mol. weight [g/mol]:	100.16
CAS:	4798-44-1

Physical Properties

Property code	Value	Unit	Source
gf	-51.78	kJ/mol	Joback Method
hf	-199.25	kJ/mol	Joback Method
hfus	10.58	kJ/mol	Joback Method
hvap	44.57	kJ/mol	Joback Method
log10ws	-0.59		Aqueous Solubility Prediction Method
log10ws	-0.59		Estimated Solubility Method
logp	1.333		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
rinpol	770.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	767.00		NIST Webbook

rinpol	771.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	776.00		NIST Webbook
ripol	1295.00		NIST Webbook
ripol	1248.00		NIST Webbook
ripol	1225.00		NIST Webbook
ripol	1228.00		NIST Webbook
ripol	1254.00		NIST Webbook
ripol	1261.00		NIST Webbook
ripol	1225.00		NIST Webbook
ripol	1295.00		NIST Webbook
tb	425.10	K	Joback Method
tc	592.88	K	Joback Method
tf	201.44	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.94	J/mol×K	592.88	Joback Method
cpg	201.41	J/mol×K	453.06	Joback Method
cpg	210.23	J/mol×K	481.03	Joback Method
cpg	218.68	J/mol×K	508.99	Joback Method
cpg	226.77	J/mol×K	536.95	Joback Method
cpg	234.52	J/mol×K	564.91	Joback Method
cpg	192.23	J/mol×K	425.10	Joback Method
dvisc	0.1985438	Pa×s	201.44	Joback Method
dvisc	0.0271287	Pa×s	238.72	Joback Method
dvisc	0.0063461	Pa×s	275.99	Joback Method
dvisc	0.0020977	Pa×s	313.27	Joback Method
dvisc	0.0008774	Pa×s	350.55	Joback Method
dvisc	0.0004340	Pa×s	387.82	Joback Method
dvisc	0.0002428	Pa×s	425.10	Joback Method
pvap	0.14	kPa	283.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol

pvap	0.02	kPa	263.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.02	kPa	263.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.02	kPa	263.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.04	kPa	268.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.04	kPa	268.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.04	kPa	268.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.06	kPa	273.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol

pvap	0.06	kPa	273.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.06	kPa	273.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.09	kPa	278.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.09	kPa	278.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.09	kPa	278.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.14	kPa	283.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.14	kPa	283.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol

pvap	0.01	kPa	258.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.21	kPa	288.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.21	kPa	288.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.21	kPa	288.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.31	kPa	293.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.31	kPa	293.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.31	kPa	293.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol

pvap	0.46	kPa	298.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.46	kPa	298.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.46	kPa	298.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.66	kPa	303.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.66	kPa	303.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.66	kPa	303.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.94	kPa	308.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol

pvap	0.94	kPa	308.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.94	kPa	308.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.01	kPa	258.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	0.01	kPa	258.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	7.38e-03	kPa	253.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	7.37e-03	kPa	253.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	7.37e-03	kPa	253.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol

pvap	4.19e-03	kPa	248.20	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	4.19e-03	kPa	248.20	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	4.18e-03	kPa	248.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	2.31e-03	kPa	243.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	2.31e-03	kPa	243.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	2.31e-03	kPa	243.15	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	1.25e-03	kPa	238.20	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol

pvap	1.25e-03	kPa	238.20	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol
pvap	1.24e-03	kPa	238.20	Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41423e+01
Coeff. B	-3.53631e+03
Coeff. C	-5.44770e+01
Temperature range (K), min.	295.70
Temperature range (K), max.	454.93

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4798441&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
Vapor pressures and thermophysical properties of selected hexenols and recommended vapor pressure for hexan-1-ol:	https://www.doi.org/10.1016/j.fluid.2015.05.026

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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