2,4-Hexadien-1-ol

Other names:	1-Hydroxy-2,4-hexadiene
	2,4-Hexadiene-1-ol
	2,4-Hexadienol
	Hexacose
	Hexakose
	Sorbic alcohol
	Sorbinic alcohol
	Sorbyl alcohol
	hexa-2,4-dien-1-ol
	n-Hexa-2,4-dien-1-ol
Inchi:	InChI=1S/C6H10O/c1-2-3-4-5-6-7/h2-5,7H,6H2,1H3
InchiKey:	MEIRRNXMZYDVDW-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	CC=CC=CCO
Mol. weight [g/mol]:	98.14
CAS:	111-28-4

Physical Properties

Property code	Value	Unit	Source
gf	23.26	kJ/mol	Joback Method
hf	-84.96	kJ/mol	Joback Method
hfus	15.79	kJ/mol	Joback Method
hvap	45.55	kJ/mol	Joback Method
log10ws	-1.30		Crippen Method
logp	1.111		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
rinpol	891.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	882.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1570.00		NIST Webbook
tb	437.18	K	Joback Method
tc	614.05	K	Joback Method
tf	302.00 ± 2.00	K	NIST Webbook

vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.67	J/mol×K	437.18	Joback Method
cpg	184.40	J/mol×K	466.66	Joback Method
cpg	192.67	J/mol×K	496.14	Joback Method
cpg	200.49	J/mol×K	525.62	Joback Method
cpg	207.90	J/mol×K	555.09	Joback Method
cpg	214.91	J/mol×K	584.57	Joback Method
cpg	221.56	J/mol×K	614.05	Joback Method
dvisc	0.0989187	Pa×s	208.04	Joback Method
dvisc	0.0148070	Pa×s	246.23	Joback Method
dvisc	0.0036911	Pa×s	284.42	Joback Method
dvisc	0.0012784	Pa×s	322.61	Joback Method
dvisc	0.0005542	Pa×s	360.80	Joback Method
dvisc	0.0002820	Pa×s	398.99	Joback Method
dvisc	0.0001614	Pa×s	437.18	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56104e+01
Coeff. B	-3.88524e+03
Coeff. C	-5.33670e+01
Temperature range (K), min.	306.93
Temperature range (K), max.	430.62

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C111284&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
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