

OCT-1-EN-3-OL

Other names:	1-Octene-3-ol
	1-Okten-3-ol
	1-Vinylhexanol
	1-octen-3-ol
	3-Octenol
	3-hydroxy-1-octene
	Amyl vinyl carbinol
	Flowtron mosquito attractant
	Matsuika alcohol
	Matsuka alcohol
	Matsutake alcohol
	Morillol
	Mushroom alcohol
	NSC 87563
	Oct-1-ene-3-ol
	Octen-3-ol
	Octene-1-ol-3
	Pentyl vintyl carbinol
	Pentyl vinyl carbinol
	Vinyl amyl carbinol
	Vinyl hexanol
	Vinyl pentyl carbinol
	n-Oct-1-en-3-ol
Inchi:	InChI=1S/C8H16O/c1-3-5-6-7-8(9)4-2/h4,8-9H,2-3,5-7H2,1H3
InchiKey:	VSMOENVRRABVKN-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	C=CC(O)CCCC
Mol. weight [g/mol]:	128.21
CAS:	3391-86-4

Physical Properties

Property code	Value	Unit	Source
af	0.6051		Cheméo Relay (1.0)
gf	-34.94	kJ/mol	Joback Method
hf	-278.07	kJ/mol	Cheméo Relay (1.0)
hfus	15.76	kJ/mol	Joback Method

hvap	58.86	kJ/mol	Cheméo Relay (1.0)
ie	9.61	eV	Cheméo Relay (1.0)
log10ws	-1.62		Cheméo Relay (1.0)
logp	2.114		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
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tb	441.75	K	Cheméo Relay (1.0)
tc	617.54	K	Cheméo Relay (1.0)
tf	243.67	K	Cheméo Relay (1.0)
vc	0.462	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	273.08	J/mol×K	470.86	Joback Method
cpg	284.36	J/mol×K	498.51	Joback Method
cpg	295.19	J/mol×K	526.16	Joback Method
cpg	305.56	J/mol×K	553.81	Joback Method
cpg	315.50	J/mol×K	581.46	Joback Method
cpg	325.02	J/mol×K	609.11	Joback Method
cpg	334.14	J/mol×K	636.76	Joback Method
dvisc	0.1097275	Pa×s	223.98	Joback Method
dvisc	0.0162547	Pa×s	265.13	Joback Method
dvisc	0.0040223	Pa×s	306.27	Joback Method
dvisc	0.0013856	Pa×s	347.42	Joback Method
dvisc	0.0005982	Pa×s	388.57	Joback Method
dvisc	0.0003033	Pa×s	429.71	Joback Method
dvisc	0.0001732	Pa×s	470.86	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.36175e+01
Coeff. B	-3.69020e+03
Coeff. C	-6.57630e+01
Temperature range (K), min.	342.60
Temperature range (K), max.	510.04

Sources

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Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Solubility of three natural compounds with insecticidal activity in supercritical carbon dioxide: Experimental Dilution of Melarubin Compounds in Water and in the Yaws Handbook of Vapor Pressure: Pressure:

<https://www.doi.org/10.1016/j.fluid.2019.04.011>

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Cheméo Relay (1.0):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3391864&Units=SI>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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