

2-Octen-1-ol, (E)-

Other names:	(2E)-2-Octen-1-ol
	(E)-2-Octen-1-ol
	(E)-2-Octenol
	(E)-Oct-2-en-1-ol
	(E)-Oct-2-enol
	2-(E)-Octen-1-ol
	trans-1-Oct-2-enol
	trans-2-Octen-1-ol
	trans-2-Octenol
Inchi:	InChI=1S/C8H16O/c1-2-3-4-5-6-7-8-9/h6-7,9H,2-5,8H2,1H3/b7-6+
InchiKey:	AYQPVPFZWIQERS-VOTSOKGWSA-N
Formula:	C8H16O
SMILES:	CCCCC=CCO
Mol. weight [g/mol]:	128.21
CAS:	18409-17-1

Physical Properties

Property code	Value	Unit	Source
gf	-40.12	kJ/mol	Joback Method
hf	-243.46	kJ/mol	Joback Method
hfus	20.77	kJ/mol	Joback Method
hvap	50.04	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.115		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
rinpol	1059.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1067.00		NIST Webbook

rinpol	1059.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1064.00	NIST Webbook
rinpol	1055.00	NIST Webbook
rinpol	1052.00	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1071.00	NIST Webbook
rinpol	1069.00	NIST Webbook
ripol	1613.00	NIST Webbook
ripol	1590.00	NIST Webbook
ripol	1620.00	NIST Webbook
ripol	1622.00	NIST Webbook
ripol	1622.00	NIST Webbook
ripol	1611.00	NIST Webbook
ripol	1590.00	NIST Webbook
ripol	1620.00	NIST Webbook
ripol	1622.00	NIST Webbook
ripol	1622.00	NIST Webbook
ripol	1609.00	NIST Webbook
ripol	1612.00	NIST Webbook
ripol	1609.00	NIST Webbook
ripol	1612.00	NIST Webbook
ripol	1605.00	NIST Webbook
ripol	1613.00	NIST Webbook
ripol	1616.00	NIST Webbook
ripol	1616.00	NIST Webbook
ripol	1645.20	NIST Webbook
ripol	1645.20	NIST Webbook
ripol	1603.00	NIST Webbook
ripol	1611.00	NIST Webbook
ripol	1613.00	NIST Webbook
ripol	1590.00	NIST Webbook
ripol	1618.00	NIST Webbook
ripol	1615.00	NIST Webbook
ripol	1616.00	NIST Webbook
ripol	1587.00	NIST Webbook
ripol	1590.00	NIST Webbook
ripol	1620.00	NIST Webbook
ripol	1639.00	NIST Webbook
ripol	1649.00	NIST Webbook
ripol	1626.00	NIST Webbook
ripol	1603.00	NIST Webbook
ripol	1615.00	NIST Webbook

ripol	1603.00		NIST Webbook
tb	478.78	K	Joback Method
tc	645.49	K	Joback Method
tf	235.66	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.29	J/mol×K	478.78	Joback Method
cpg	324.63	J/mol×K	617.71	Joback Method
cpg	315.25	J/mol×K	589.92	Joback Method
cpg	305.44	J/mol×K	562.14	Joback Method
cpg	295.20	J/mol×K	534.35	Joback Method
cpg	284.49	J/mol×K	506.57	Joback Method
cpg	333.60	J/mol×K	645.49	Joback Method
dvisc	0.0001449	Pa×s	478.78	Joback Method
dvisc	0.0002469	Pa×s	438.26	Joback Method
dvisc	0.0004689	Pa×s	397.74	Joback Method
dvisc	0.0010300	Pa×s	357.22	Joback Method
dvisc	0.0027674	Pa×s	316.70	Joback Method
dvisc	0.0099375	Pa×s	276.18	Joback Method
dvisc	0.0553869	Pa×s	235.66	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.55989e+01
Coeff. B	-4.42976e+03
Coeff. C	-7.24080e+01
Temperature range (K), min.	361.72
Temperature range (K), max.	503.01

Sources

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=C18409171&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

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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