3-Octen-1-ol

Other names:	3-Octenol
	Oct-3-en-1-ol
	Oct-3-en-1-ol (Isomer 2)
Inchi:	InChI=1S/C8H16O/c1-2-3-4-5-6-7-8-9/h5-6,9H,2-4,7-8H2,1H3/b6-5+
InchiKey:	YDXQPTHHAPCTPP-AATRIKPKSA-N
Formula:	C8H16O
SMILES:	CCCCC=CCCO
Mol. weight [g/mol]:	128.21
CAS:	18185-81-4

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
ripol	1444.00		NIST Webbook
ripol	1444.00		NIST Webbook
ripol	1441.00		NIST Webbook
ripol	1440.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1438.00		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	284.49	J/mol×K	506.57	Joback Method
cpg	295.20	J/mol×K	534.35	Joback Method
cpg	305.44	J/mol×K	562.14	Joback Method
cpg	315.25	J/mol×K	589.92	Joback Method
cpg	324.63	J/mol×K	617.71	Joback Method
cpg	333.60	J/mol×K	645.49	Joback Method
dvisc	0.0553869	Pa×s	235.66	Joback Method
dvisc	0.0099375	Pa×s	276.18	Joback Method
dvisc	0.0027674	Pa×s	316.70	Joback Method
dvisc	0.0010300	Pa×s	357.22	Joback Method
dvisc	0.0004689	Pa×s	397.74	Joback Method
dvisc	0.0002469	Pa×s	438.26	Joback Method
dvisc	0.0001449	Pa×s	478.78	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18185814&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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