2-Octenal

Other names:	oct-2-enal
	oct-2-enal (isomer)
Inchi:	InChI=1S/C8H14O/c1-2-3-4-5-6-7-8-9/h6-8H,2-5H2,1H3
InchiKey:	LVBXEMGDVWVTGY-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	CCCCCC=CC=O
Mol. weight [g/mol]:	126.20
CAS:	2363-89-5

Physical Properties

Property code	Value	Unit	Source
gf	-2.82	kJ/mol	Joback Method
hf	-176.81	kJ/mol	Joback Method
hfus	18.97	kJ/mol	Joback Method
hvap	40.08	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1041.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1036.60		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1056.00		NIST Webbook

rinpol	1059.00	NIST Webbook
rinpol	1063.00	NIST Webbook
rinpol	1075.00	NIST Webbook
rinpol	1062.00	NIST Webbook
rinpol	1045.00	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1031.00	NIST Webbook
rinpol	1027.00	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1062.00	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1062.00	NIST Webbook
rinpol	1062.00	NIST Webbook
rinpol	1034.00	NIST Webbook
rinpol	1023.00	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1055.00	NIST Webbook
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rinpol	1055.00	NIST Webbook
ripol	1445.00	NIST Webbook
ripol	1416.00	NIST Webbook
ripol	1445.00	NIST Webbook
ripol	1427.00	NIST Webbook
ripol	1382.00	NIST Webbook
ripol	1402.00	NIST Webbook
ripol	1413.00	NIST Webbook
ripol	1421.00	NIST Webbook
ripol	1460.00	NIST Webbook
ripol	1436.00	NIST Webbook
ripol	1400.00	NIST Webbook
ripol	1378.00	NIST Webbook
ripol	1414.00	NIST Webbook

ripol	1412.00		NIST Webbook
ripol	1442.00		NIST Webbook
ripol	1440.00		NIST Webbook
ripol	1416.00		NIST Webbook
ripol	1436.00		NIST Webbook
ripol	1414.00		NIST Webbook
tb	435.26	K	Joback Method
tc	614.34	K	Joback Method
tf	216.84	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.07	J/mol×K	435.26	Joback Method
cpg	252.93	J/mol×K	465.11	Joback Method
cpg	264.25	J/mol×K	494.95	Joback Method
cpg	275.03	J/mol×K	524.80	Joback Method
cpg	285.31	J/mol×K	554.65	Joback Method
cpg	295.10	J/mol×K	584.49	Joback Method
cpg	304.43	J/mol×K	614.34	Joback Method
dvisc	0.0045537	Pa×s	216.84	Joback Method
dvisc	0.0020114	Pa×s	253.24	Joback Method
dvisc	0.0010910	Pa×s	289.65	Joback Method
dvisc	0.0006784	Pa×s	326.05	Joback Method
dvisc	0.0004641	Pa×s	362.45	Joback Method
dvisc	0.0003402	Pa×s	398.86	Joback Method
dvisc	0.0002628	Pa×s	435.26	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46514e+01
Coeff. B	-3.95760e+03
Coeff. C	-6.87940e+01
Temperature range (K), min.	344.32

Temperature range (K), max.	492.52

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=C2363895&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
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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