3-Octenal

Other names: 3-Octen-1-one
Inchi: InChI=1S/C8H14O/c1-2-3-4-5-6-7-8-9/h5-6,8H,2-4,7H2,1H3/b6-5+
InchiKey: WDWAUVJQFVTKEW-AATRIKPKSA-N
Formula: C8H14O
SMILES: CCCCC=CCC=O
Mol. weight [g/mol]: 126.20
CAS: ---

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	991.00		NIST Webbook
rinpol	991.00		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	1.51611e+01
Coeff. B	-4.09803e+03
Coeff. C	-6.87940e+01
Temperature range (K), min.	344.32
Temperature range (K), max.	484.85

Sources

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=R286265&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

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

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