2-Hexenal

Other names:	2-Hexen-1-al
	Hex-2-en-1-al
	Hex-2-enal
	Hexylenic aldehyde
	Leaf aldehyde
	n-C3H7CH=CHCHO
Inchi:	InChI=1S/C6H10O/c1-2-3-4-5-6-7/h4-6H,2-3H2,1H3
InchiKey:	MBDOYVRWFFCFHM-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	CCCC=CC=O
Mol. weight [g/mol]:	98.14
CAS:	505-57-7

Physical Properties

Property code	Value	Unit	Source
gf	-19.66	kJ/mol	Joback Method
hf	-135.53	kJ/mol	Joback Method
hfus	13.79	kJ/mol	Joback Method
hvap	35.63	kJ/mol	Joback Method
ie	9.65	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	825.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	817.00		NIST Webbook

rinpol	816.00	NIST Webbook
rinpol	824.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	824.00	NIST Webbook
rinpol	851.00	NIST Webbook
rinpol	847.00	NIST Webbook
rinpol	854.00	NIST Webbook
rinpol	850.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	840.00	NIST Webbook
rinpol	832.00	NIST Webbook
rinpol	832.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	854.00	NIST Webbook
rinpol	857.00	NIST Webbook
rinpol	854.00	NIST Webbook
rinpol	850.00	NIST Webbook
rinpol	860.00	NIST Webbook
rinpol	860.00	NIST Webbook
rinpol	848.00	NIST Webbook
rinpol	841.00	NIST Webbook
rinpol	862.00	NIST Webbook
rinpol	838.00	NIST Webbook
rinpol	854.00	NIST Webbook
rinpol	828.70	NIST Webbook
rinpol	851.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	839.00	NIST Webbook
rinpol	832.00	NIST Webbook
rinpol	823.00	NIST Webbook
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rinpol	856.00	NIST Webbook
rinpol	843.00	NIST Webbook
rinpol	839.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	850.00	NIST Webbook
rinpol	852.00	NIST Webbook
rinpol	841.00	NIST Webbook
rinpol	811.00	NIST Webbook
rinpol	832.00	NIST Webbook
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rinpol	848.00		NIST Webbook
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rinpol	857.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	823.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1178.00		NIST Webbook
ripol	1212.00		NIST Webbook
ripol	1213.00		NIST Webbook
ripol	1216.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1230.00		NIST Webbook
ripol	1213.00		NIST Webbook
ripol	1230.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1201.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1226.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1216.00		NIST Webbook
ripol	1216.00		NIST Webbook
ripol	1220.00		NIST Webbook
ripol	1248.00		NIST Webbook
ripol	1225.00		NIST Webbook
tb	389.50	K	Joback Method
tc	570.95	K	Joback Method
tf	194.30	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.69	J/mol×K	389.50	Joback Method
cpg	174.16	J/mol×K	419.74	Joback Method
cpg	183.18	J/mol×K	449.98	Joback Method
cpg	191.76	J/mol×K	480.23	Joback Method
cpg	199.93	J/mol×K	510.47	Joback Method
cpg	207.70	J/mol×K	540.71	Joback Method
cpg	215.09	J/mol×K	570.95	Joback Method
dvisc	0.0038680	Pa×s	194.30	Joback Method
dvisc	0.0017894	Pa×s	226.83	Joback Method
dvisc	0.0010044	Pa×s	259.37	Joback Method
dvisc	0.0006413	Pa×s	291.90	Joback Method
dvisc	0.0004480	Pa×s	324.43	Joback Method
dvisc	0.0003341	Pa×s	356.97	Joback Method
dvisc	0.0002617	Pa×s	389.50	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63489e+01
Coeff. B	-4.09415e+03
Coeff. C	-5.78130e+01
Temperature range (K), min.	312.72
Temperature range (K), max.	428.75

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C505577&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

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

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
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