3-Hexenal

Other names:	Hex-3-enal
Inchi:	InChI=1S/C6H10O/c1-2-3-4-5-6-7/h3-4,6H,2,5H2,1H3/b4-3+
InchiKey:	GXANMBISFKBPEX-ONEGZZNKSA-N
Formula:	C6H10O
SMILES:	CCC=CCC=O
Mol. weight [g/mol]:	98.14
CAS:	4440-65-7

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
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	769.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	802.70		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	818.00		NIST Webbook
ripol	1146.00		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	1.43248e+01
Coeff. B	-3.43895e+03
Coeff. C	-5.25310e+01
Temperature range (K), min.	297.52
Temperature range (K), max.	434.07

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=C4440657&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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