

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	773.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	802.70		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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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