

3-Hexenal, (z)-

Other names:	(3Z)-3-Hexenal (Z)-3-Hexen-1-al (Z)-3-Hexenal (Z)-Hex-3enal 3-(Z)-Hexenal Hex-cis-3-enal cis-3-Hexenal cis-«beta»,«gamma»-Hexylenic aldehyde
Inchi:	InChI=1S/C6H10O/c1-2-3-4-5-6-7/h3-4,6H,2,5H2,1H3
InchiKey:	GXANMBISFKBPEX-ARJAWSKDSA-N
Formula:	C6H10O
SMILES:	CC/C=C\CC=O
Mol. weight [g/mol]:	98.14
CAS:	6789-80-6

Physical Properties

Property code	Value	Unit	Source
af	0.3134		Cheméo Relay (1.0)
gf	-19.66	kJ/mol	Joback Method
hf	-164.83	kJ/mol	Cheméo Relay (1.0)
hfus	13.79	kJ/mol	Joback Method
hvap	40.29	kJ/mol	Cheméo Relay (1.0)
ie	9.38	eV	Cheméo Relay (1.0)
log10ws	-1.09		Cheméo Relay (1.0)
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	770.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	800.00		NIST Webbook
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rinpol	800.00	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	803.00	NIST Webbook
rinpol	796.00	NIST Webbook
rinpol	799.00	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	775.00	NIST Webbook
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ripol	1153.00		NIST Webbook
ripol	1135.00		NIST Webbook
ripol	1142.00		NIST Webbook
ripol	1138.00		NIST Webbook
tb	398.84	K	Cheméo Relay (1.0)
tc	585.17	K	Cheméo Relay (1.0)
tf	189.75	K	Cheméo Relay (1.0)
vc	0.328	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37556e+01
Coeff. B	-3.25383e+03
Coeff. C	-5.07240e+01
Temperature range (K), min.	292.32
Temperature range (K), max.	436.06

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6789806&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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

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