

2-Hexenal, (E)-

Other names:	(2E)-2-Hexenal (E)-2-Hexanal (E)-2-Hexen-1-al (E)-2-Hexenal (E)-Hex-2-en-1-al (E)-Hex-2-enal 2-(E)-Hexenal 2-Hexenal, (2E)- 2-trans-Hexenal Hex-2(E)-enal Hex-trans-2-enal Leaf aldehyde n-Hex-trans-2-enal t-2-Hexenal trans-2-Hexen-1-al trans-2-Hexenal trans-Hex-2-enal
Inchi:	InChI=1S/C6H10O/c1-2-3-4-5-6-7/h4-6H,2-3H2,1H3/b5-4+
InchiKey:	MBDOYVRWFFCFHM-SNAWJCMRSA-N
Formula:	C6H10O
SMILES:	CCCC=CC=O
Mol. weight [g/mol]:	98.14
CAS:	6728-26-3

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
mcpvol	92.670	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
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ripol	1230.00		NIST Webbook
ripol	1228.00		NIST Webbook
ripol	1221.00		NIST Webbook
ripol	1212.00		NIST Webbook
tb	419.70	K	NIST Webbook
tb	420.70	K	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
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
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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	373.50	K	24.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	383.00	K	34.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	390.40	K	43.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	396.90	K	53.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	402.60	K	62.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa

tbp	407.70	K	72.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	412.00	K	81.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	416.10	K	91.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	423.80	K	110.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	427.10	K	119.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	430.30	K	129.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	433.10	K	138.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa

tbp	435.90	K	148.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	438.40	K	157.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	441.00	K	167.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	443.40	K	176.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	445.40	K	186.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	446.20	K	190.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbrp	320.20	K	2.30	NIST Webbook
tbrp	316.20	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49374e+01
Coeff. B	-3.73435e+03
Coeff. C	-5.78130e+01
Temperature range (K), min.	312.72
Temperature range (K), max.	445.76

Sources

Vapor pressure data for ethyl-2-methylbutyrate, hexanal and ethyl-hexanoate at a pressure range of (25 to 1013.25) kPa for ternary systems ethyl-2-methylbutyrate (E)-2-hexenal or hexanal + carbon dioxide + water): Partition Coefficient Measurement:	https://www.doi.org/10.1016/j.jct.2014.03.006
NIST Webbook:	https://www.doi.org/10.1016/j.jct.2015.05.003
The Yaws Handbook of Vapor Pressure:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6728263&Units=SI
Crippen Method:	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

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
tbp:	Boiling point at given pressure
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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