

3-Hexenoic acid, (E)-

Other names:	(E)-3-Hexenoic acid 3(E)-hexenoic acid 3-Hexenoic acid, (3E)- trans-3-Hexenoic Acid trans-Hex-3-enoic acid
Inchi:	InChI=1S/C6H10O2/c1-2-3-4-5-6(7)8/h3-4H,2,5H2,1H3,(H,7,8)/b4-3+
InchiKey:	XXHDAWYDNSXJQM-ONEGZZNKSA-N
Formula:	C6H10O2
SMILES:	CCC=CCC(=O)O
Mol. weight [g/mol]:	114.14
CAS:	1577-18-0

Physical Properties

Property code	Value	Unit	Source
gf	-185.88	kJ/mol	Joback Method
hf	-314.76	kJ/mol	Joback Method
hfus	17.19	kJ/mol	Joback Method
hvap	52.33	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.427		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
ripol	1021.00		NIST Webbook
ripol	1021.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1957.00		NIST Webbook
ripol	1929.00		NIST Webbook
ripol	1909.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1924.00		NIST Webbook
ripol	1948.00		NIST Webbook
tb	486.89	K	Joback Method
tc	665.94	K	Joback Method
tf	263.05	K	Joback Method
vc	0.377	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.08	J/molxK	486.89	Joback Method
cpg	214.50	J/molxK	516.73	Joback Method
cpg	222.51	J/molxK	546.57	Joback Method
cpg	230.13	J/molxK	576.41	Joback Method
cpg	237.37	J/molxK	606.26	Joback Method
cpg	244.26	J/molxK	636.10	Joback Method
cpg	250.80	J/molxK	665.94	Joback Method
dvisc	0.0232383	Paxs	263.05	Joback Method
dvisc	0.0061439	Paxs	300.36	Joback Method
dvisc	0.0021795	Paxs	337.66	Joback Method
dvisc	0.0009502	Paxs	374.97	Joback Method
dvisc	0.0004814	Paxs	412.28	Joback Method
dvisc	0.0002731	Paxs	449.58	Joback Method
dvisc	0.0001689	Paxs	486.89	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	391.70	K	2.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49002e+01
Coeff. B	-4.26704e+03
Coeff. C	-7.49100e+01
Temperature range (K), min.	366.92
Temperature range (K), max.	519.91

Sources

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=C1577180&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

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

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