

2-Hexenoic acid

Other names:	Hex-2-enoic acid
Inchi:	InChI=1S/C6H10O2/c1-2-3-4-5-6(7)8/h4-5H,2-3H2,1H3,(H,7,8)/b5-4+
InchiKey:	NIONDZDPPYHYKY-SNAWJCMRSA-N
Formula:	C6H10O2
SMILES:	CCCC=CC(=O)O
Mol. weight [g/mol]:	114.14
CAS:	1191-04-4

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	1980.00		NIST Webbook
ripol	1984.00		NIST Webbook
tb	486.89	K	Joback Method
tc	665.94	K	Joback Method
tf	263.05	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.08	J/molxK	486.89	Joback Method
cpg	244.26	J/molxK	636.10	Joback Method
cpg	237.37	J/molxK	606.26	Joback Method
cpg	230.13	J/molxK	576.41	Joback Method
cpg	222.51	J/molxK	546.57	Joback Method
cpg	214.50	J/molxK	516.73	Joback Method

cpg	250.80	J/mol×K	665.94	Joback Method
dvisc	0.0001689	Paxs	486.89	Joback Method
dvisc	0.0002731	Paxs	449.58	Joback Method
dvisc	0.0004814	Paxs	412.28	Joback Method
dvisc	0.0009502	Paxs	374.97	Joback Method
dvisc	0.0021795	Paxs	337.66	Joback Method
dvisc	0.0061439	Paxs	300.36	Joback Method
dvisc	0.0232383	Paxs	263.05	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56450e+01
Coeff. B	-4.55266e+03
Coeff. C	-7.72730e+01
Temperature range (K), min.	373.72
Temperature range (K), max.	517.84

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1191044&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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