3-Hexenoic acid

Other names: Hex-3-enoic acid
Hydrosorbic acid
Inchi: InChI=1S/C6H10O2/c1-2-3-4-5-6(7)8/h3-4H,2,5H2,1H3,(H,7,8)
InchiKey: XXHDAWYDNSXJQM-UHFFFAOYSA-N
Formula: C6H10O2
SMILES: CCC=CCC(=O)O
Mol. weight [g/mol]: 114.14
CAS: 4219-24-3

Physical Properties

Property code	Value	Unit	Source
chl	-3338.00	kJ/mol	NIST Webbook
chl	-3342.10	kJ/mol	NIST Webbook
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
rinpol	983.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	983.00		NIST Webbook
ripol	1954.00		NIST Webbook
ripol	1954.00		NIST Webbook
ripol	1977.00		NIST Webbook
ripol	1977.00		NIST Webbook
tb	481.20	K	NIST Webbook
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/mol×K	486.89	Joback Method
cpg	244.26	J/mol×K	636.10	Joback Method
cpg	237.37	J/mol×K	606.26	Joback Method
cpg	230.13	J/mol×K	576.41	Joback Method
cpg	222.51	J/mol×K	546.57	Joback Method
cpg	214.50	J/mol×K	516.73	Joback Method
cpg	250.80	J/mol×K	665.94	Joback Method
dvisc	0.0001689	Pa×s	486.89	Joback Method
dvisc	0.0002731	Pa×s	449.58	Joback Method
dvisc	0.0004814	Pa×s	412.28	Joback Method
dvisc	0.0009502	Pa×s	374.97	Joback Method
dvisc	0.0021795	Pa×s	337.66	Joback Method
dvisc	0.0061439	Pa×s	300.36	Joback Method
dvisc	0.0232383	Pa×s	263.05	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56843e+01
Coeff. B	-4.49600e+03
Coeff. C	-7.49100e+01
Temperature range (K), min.	366.92
Temperature range (K), max.	508.35

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C4219243&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume