5-Hexenoic acid

Other names: Hex-5-enoic acid
Inchi: InChI=1S/C6H10O2/c1-2-3-4-5-6(7)8/h2H,1,3-5H2,(H,7,8)
InchiKey: XUDOZULIAWNMIU-UHFFFAOYSA-N
Formula: C6H10O2
SMILES: C=CCCCC(=O)O
Mol. weight [g/mol]: 114.14
CAS: 1577-22-6

Physical Properties

Property code	Value	Unit	Source
gf	-178.26	kJ/mol	Joback Method
hf	-306.55	kJ/mol	Joback Method
hfus	15.70	kJ/mol	Joback Method
hvap	51.70	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.427		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
ripol	1885.00		NIST Webbook
ripol	1885.00		NIST Webbook
tb	479.41	K	Joback Method
tc	654.04	K	Joback Method
tf	266.37	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.60	J/mol×K	479.41	Joback Method
cpg	214.87	J/mol×K	508.52	Joback Method
cpg	222.77	J/mol×K	537.62	Joback Method
cpg	230.31	J/mol×K	566.73	Joback Method
cpg	237.50	J/mol×K	595.83	Joback Method
cpg	244.37	J/mol×K	624.94	Joback Method

cpg	250.90	J/mol×K	654.04	Joback Method
dvisc	0.0217559	Pa×s	266.37	Joback Method
dvisc	0.0063859	Pa×s	301.88	Joback Method
dvisc	0.0024261	Pa×s	337.38	Joback Method
dvisc	0.0011083	Pa×s	372.89	Joback Method
dvisc	0.0005802	Pa×s	408.40	Joback Method
dvisc	0.0003368	Pa×s	443.90	Joback Method
dvisc	0.0002120	Pa×s	479.41	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44874e+01
Coeff. B	-4.10942e+03
Coeff. C	-7.35200e+01
Temperature range (K), min.	362.92
Temperature range (K), max.	521.37

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=C1577226&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/ci990307l

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