cis-3-Hexenoic acid

Other names: (Z)-3-hexenoic acid
(Z)-hex-2-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-ARJAWSKDSA-N
Formula: C6H10O2
SMILES: CCC=CCC(=O)O
Mol. weight [g/mol]: 114.14
CAS: 1775-43-5

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
rinpol	1101.00		NIST Webbook
ripol	1945.00		NIST Webbook
ripol	1922.00		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/mol×K	486.89	Joback Method
cpg	214.50	J/mol×K	516.73	Joback Method
cpg	222.51	J/mol×K	546.57	Joback Method
cpg	230.13	J/mol×K	576.41	Joback Method

cpg	237.37	J/mol×K	606.26	Joback Method
cpg	244.26	J/mol×K	636.10	Joback Method
cpg	250.80	J/mol×K	665.94	Joback Method
dvisc	0.0232383	Pa×s	263.05	Joback Method
dvisc	0.0061439	Pa×s	300.36	Joback Method
dvisc	0.0021795	Pa×s	337.66	Joback Method
dvisc	0.0009502	Pa×s	374.97	Joback Method
dvisc	0.0004814	Pa×s	412.28	Joback Method
dvisc	0.0002731	Pa×s	449.58	Joback Method
dvisc	0.0001689	Pa×s	486.89	Joback Method

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=C1775435&Units=SI
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
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