Hexanal, 4-methyl-

Other names: 4-methylhexanal
Inchi: InChI=1S/C7H14O/c1-3-7(2)5-4-6-8/h6-7H,3-5H2,1-2H3
InchiKey: GIGNTOMJQYNUNL-UHFFFAOYSA-N
Formula: C7H14O
SMILES: CCC(C)CCC=O
Mol. weight [g/mol]: 114.19
CAS: 41065-97-8

Physical Properties

Property code	Value	Unit	Source
gf	-93.90	kJ/mol	Joback Method
hf	-278.67	kJ/mol	Joback Method
hfus	12.65	kJ/mol	Joback Method
hvap	37.51	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	2.012		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	889.00		NIST Webbook
rinpol	889.00		NIST Webbook
tb	407.78	K	Joback Method
tc	583.42	K	Joback Method
tf	195.65	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.97	J/mol×K	407.78	Joback Method
cpg	228.33	J/mol×K	437.05	Joback Method
cpg	239.24	J/mol×K	466.33	Joback Method
cpg	249.71	J/mol×K	495.60	Joback Method
cpg	259.76	J/mol×K	524.87	Joback Method
cpg	269.38	J/mol×K	554.14	Joback Method

cpg	278.60	J/mol×K	583.42	Joback Method
dvisc	0.0075086	Pa×s	195.65	Joback Method
dvisc	0.0029368	Pa×s	231.00	Joback Method
dvisc	0.0014738	Pa×s	266.36	Joback Method
dvisc	0.0008693	Pa×s	301.72	Joback Method
dvisc	0.0005728	Pa×s	337.07	Joback Method
dvisc	0.0004085	Pa×s	372.42	Joback Method
dvisc	0.0003089	Pa×s	407.78	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53879e+01
Coeff. B	-3.88290e+03
Coeff. C	-5.63390e+01
Temperature range (K), min.	313.48
Temperature range (K), max.	441.68

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=C41065978&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume