4-Methyl-2-pentenal

Inchi: InChI=1S/C6H10O/c1-6(2)4-3-5-7/h3-6H,1-2H3/b4-3+
InchiKey: RIWPMNBTULNXOH-ONEGZZNKSA-N
Formula: C6H10O
SMILES: CC(C)C=CC=O
Mol. weight [g/mol]: 98.14
CAS: 5362-56-1

Physical Properties

Property code	Value	Unit	Source
gf	-22.10	kJ/mol	Joback Method
hf	-140.81	kJ/mol	Joback Method
hfus	10.26	kJ/mol	Joback Method
hvap	35.24	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.397		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
ripol	1095.00		NIST Webbook
ripol	1095.00		NIST Webbook
tb	389.06	K	Joback Method
tc	574.87	K	Joback Method
tf	179.30	K	Joback Method
vc	0.362	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.65	J/mol×K	389.06	Joback Method
cpg	209.01	J/mol×K	543.90	Joback Method
cpg	201.02	J/mol×K	512.93	Joback Method
cpg	192.61	J/mol×K	481.96	Joback Method
cpg	183.76	J/mol×K	451.00	Joback Method
cpg	174.45	J/mol×K	420.03	Joback Method
cpg	216.59	J/mol×K	574.87	Joback Method

dvisc	0.0002530	Pa×s	389.06	Joback Method
dvisc	0.0003329	Pa×s	354.10	Joback Method
dvisc	0.0004653	Pa×s	319.14	Joback Method
dvisc	0.0007061	Pa×s	284.18	Joback Method
dvisc	0.0012046	Pa×s	249.22	Joback Method
dvisc	0.0024463	Pa×s	214.26	Joback Method
dvisc	0.0065488	Pa×s	179.30	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43708e+01
Coeff. B	-3.45391e+03
Coeff. C	-5.26700e+01
Temperature range (K), min.	297.92
Temperature range (K), max.	433.92

Sources

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=R593449&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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