4-Pentenal

Other names: Pent-4-enal
Inchi: InChI=1S/C5H8O/c1-2-3-4-5-6/h2,5H,1,3-4H2
InchiKey: QUMSUJWRUHPEEJ-UHFFFAOYSA-N
Formula: C5H8O
SMILES: C=CCCC=O
Mol. weight [g/mol]: 84.12
CAS: 2100-17-6

Physical Properties

Property code	Value	Unit	Source
gf	-20.46	kJ/mol	Joback Method
hf	-106.68	kJ/mol	Joback Method
hfus	9.71	kJ/mol	Joback Method
hvap	32.77	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.151		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
rinpol	820.00		NIST Webbook
rinpol	820.00		NIST Webbook
ripol	1134.00		NIST Webbook
ripol	1123.00		NIST Webbook
tb	359.14	K	Joback Method
tc	535.69	K	Joback Method
tf	183.20 ± 0.60	K	NIST Webbook
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	131.25	J/mol×K	359.14	Joback Method
cpg	138.97	J/mol×K	388.57	Joback Method
cpg	146.37	J/mol×K	417.99	Joback Method
cpg	153.45	J/mol×K	447.42	Joback Method

cpg	160.21	J/mol×K	476.84	Joback Method
cpg	166.68	J/mol×K	506.27	Joback Method
cpg	172.86	J/mol×K	535.69	Joback Method
dvisc	0.0030720	Pa×s	186.35	Joback Method
dvisc	0.0015994	Pa×s	215.15	Joback Method
dvisc	0.0009714	Pa×s	243.95	Joback Method
dvisc	0.0006555	Pa×s	272.75	Joback Method
dvisc	0.0004769	Pa×s	301.54	Joback Method
dvisc	0.0003667	Pa×s	330.34	Joback Method
dvisc	0.0002941	Pa×s	359.14	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43066e+01
Coeff. B	-3.22594e+03
Coeff. C	-4.46080e+01
Temperature range (K), min.	274.72
Temperature range (K), max.	403.24

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=C2100176&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume