Pentanal, 2-methyl-

Other names:	2-Formylpentane
	2-Methyl-n-valeraldehyde
	2-Methylpental
	2-Methylpentaldehyde
	2-Methylpentanal
	2-Methylvaleraldehyde
	2-Methylvaleric aldehyde
	NSC 49351
	UN 2367
	Valeraldehyde, 2-methyl-
	n-C3H7CH(CH3)CHO
	«alpha»-Methyl valeraldehyde
	«alpha»-Methylpentanal
	Â«alphaÂ»-Methyl valeraldehyde
	Â«alphaÂ»-Methylpentanal
Inchi:	InChI=1S/C6H12O/c1-3-4-6(2)5-7/h5-6H,3-4H2,1-2H3
InchiKey:	FTZILAQGHINQQR-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CCCC(C)C=O
Mol. weight [g/mol]:	100.16
CAS:	123-15-9

Physical Properties

Property code	Value	Unit	Source
gf	-102.32	kJ/mol	Joback Method
hf	-258.03	kJ/mol	Joback Method
hfus	10.06	kJ/mol	Joback Method
hvap	35.28	kJ/mol	Joback Method
ie	9.70	eV	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.621		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
rinpol	746.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	791.00		NIST Webbook

rinpol	760.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	736.00		NIST Webbook
rinpol	745.80		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	740.00		NIST Webbook
rinpol	745.80		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	736.00		NIST Webbook
tb	384.90	K	Joback Method
tc	561.39	K	Joback Method
tf	184.38	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.50	J/mol×K	384.90	Joback Method
cpg	189.59	J/mol×K	414.32	Joback Method
cpg	199.28	J/mol×K	443.73	Joback Method
cpg	208.60	J/mol×K	473.15	Joback Method
cpg	217.54	J/mol×K	502.56	Joback Method
cpg	226.11	J/mol×K	531.98	Joback Method
cpg	234.32	J/mol×K	561.39	Joback Method
dvisc	0.0070161	Pa×s	184.38	Joback Method
dvisc	0.0027952	Pa×s	217.80	Joback Method
dvisc	0.0014226	Pa×s	251.22	Joback Method
dvisc	0.0008484	Pa×s	284.64	Joback Method
dvisc	0.0005641	Pa×s	318.06	Joback Method
dvisc	0.0004053	Pa×s	351.48	Joback Method
dvisc	0.0003084	Pa×s	384.90	Joback Method

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55136e+01
Coeff. B	-3.72256e+03
Coeff. C	-4.93340e+01
Temperature range (K), min.	293.82
Temperature range (K), max.	414.21

Sources

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
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=C123159&Units=SI

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
ie:	Ionization energy
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