2,3-Dimethylpentanal

Other names:	2,3-Dimethylpentaldehyde
	2,3-Dimethylvaleraldehyde
	Butanal, 3-ethyl-2-methyl
	Valeraldehyde, 2,3-dimethyl-
Inchi:	InChI=1S/C7H14O/c1-4-6(2)7(3)5-8/h5-7H,4H2,1-3H3
InchiKey:	BOHKXQAJUVXBDQ-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CCC(C)C(C)C=O
Mol. weight [g/mol]:	114.19
CAS:	32749-94-3

Physical Properties

Property code	Value	Unit	Source
af	0.3742		Cheméo Relay (1.0)
gf	-96.34	kJ/mol	Joback Method
hf	-288.80	kJ/mol	Cheméo Relay (1.0)
hfus	9.13	kJ/mol	Joback Method
hvap	42.58	kJ/mol	Cheméo Relay (1.0)
ie	9.46	eV	Cheméo Relay (1.0)
log10ws	-1.77		Cheméo Relay (1.0)
logp	1.868		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
ripol	1258.00		NIST Webbook
ripol	1258.00		NIST Webbook
tb	396.67	K	Cheméo Relay (1.0)
tc	591.87	K	Cheméo Relay (1.0)
tf	218.79	K	Cheméo Relay (1.0)
vc	0.387	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.96	J/mol×K	407.34	Joback Method

cpg	228.67	J/mol×K	437.29	Joback Method
cpg	239.91	J/mol×K	467.24	Joback Method
cpg	250.68	J/mol×K	497.19	Joback Method
cpg	260.99	J/mol×K	527.14	Joback Method
cpg	270.87	J/mol×K	557.09	Joback Method
cpg	280.30	J/mol×K	587.04	Joback Method
dvisc	0.0134730	Pa×s	180.65	Joback Method
dvisc	0.0041185	Pa×s	218.43	Joback Method
dvisc	0.0017858	Pa×s	256.21	Joback Method
dvisc	0.0009598	Pa×s	294.00	Joback Method
dvisc	0.0005942	Pa×s	331.78	Joback Method
dvisc	0.0004058	Pa×s	369.56	Joback Method
dvisc	0.0002974	Pa×s	407.34	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47179e+01
Coeff. B	-3.66015e+03
Coeff. C	-5.44770e+01
Temperature range (K), min.	308.12
Temperature range (K), max.	443.59

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C32749943&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume