4-Pentenal, 2,2-dimethyl-

Other names: 2,2-Dimethyl-4-pentenal
2,2-dimethylpent-4-enal
Inchi: InChI=1S/C7H12O/c1-4-5-7(2,3)6-8/h4,6H,1,5H2,2-3H3
InchiKey: DXSDIWHOOOBQTJ-UHFFFAOYSA-N
Formula: C7H12O
SMILES: C=CCC(C)(C)C=O
Mol. weight [g/mol]: 112.17
CAS: 5497-67-6

Physical Properties

Property code	Value	Unit	Source
gf	-0.78	kJ/mol	Joback Method
hf	-156.71	kJ/mol	Joback Method
hfus	7.48	kJ/mol	Joback Method
hvap	35.93	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.788		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
tb	397.70	K	NIST Webbook
tc	588.60	K	Joback Method
tf	211.31	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.81	J/mol×K	401.67	Joback Method
cpg	215.58	J/mol×K	432.83	Joback Method
cpg	226.70	J/mol×K	463.98	Joback Method
cpg	237.19	J/mol×K	495.14	Joback Method
cpg	247.08	J/mol×K	526.29	Joback Method
cpg	256.40	J/mol×K	557.45	Joback Method
cpg	265.18	J/mol×K	588.60	Joback Method

dvisc	0.0069011	Pa×s	211.31	Joback Method
dvisc	0.0030203	Pa×s	243.04	Joback Method
dvisc	0.0015998	Pa×s	274.76	Joback Method
dvisc	0.0009665	Pa×s	306.49	Joback Method
dvisc	0.0006418	Pa×s	338.22	Joback Method
dvisc	0.0004572	Pa×s	369.94	Joback Method
dvisc	0.0003436	Pa×s	401.67	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.29948e+01
Coeff. B	-3.16952e+03
Coeff. C	-5.48940e+01
Temperature range (K), min.	304.32
Temperature range (K), max.	467.41

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=C5497676&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume