4-Pentenal, 2-methyl-

Other names: 2-Methyl-4-pentenal
Inchi: InChI=1S/C6H10O/c1-3-4-6(2)5-7/h3,5-6H,1,4H2,2H3
InchiKey: RCQKLWAPRHHRNN-UHFFFAOYSA-N
Formula: C6H10O
SMILES: C=CCC(C)C=O
Mol. weight [g/mol]: 98.14
CAS: 5187-71-3

Physical Properties

Property code	Value	Unit	Source
gf	-14.48	kJ/mol	Joback Method
hf	-132.60	kJ/mol	Joback Method
hfus	8.78	kJ/mol	Joback Method
hvap	34.61	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.397		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
rinpol	776.30		NIST Webbook
rinpol	776.30		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	798.00		NIST Webbook
ripol	1141.00		NIST Webbook
ripol	1141.00		NIST Webbook
ripol	1141.00		NIST Webbook
ripol	1141.00		NIST Webbook
tb	381.58	K	Joback Method
tc	561.84	K	Joback Method
tf	182.62	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	165.34	J/mol×K	381.58	Joback Method
cpg	208.56	J/mol×K	531.79	Joback Method
cpg	200.69	J/mol×K	501.75	Joback Method
cpg	192.45	J/mol×K	471.71	Joback Method
cpg	183.82	J/mol×K	441.67	Joback Method
cpg	174.78	J/mol×K	411.62	Joback Method
cpg	216.06	J/mol×K	561.84	Joback Method
dvisc	0.0002995	Pa×s	381.58	Joback Method
dvisc	0.0003883	Pa×s	348.42	Joback Method
dvisc	0.0005317	Pa×s	315.26	Joback Method
dvisc	0.0007837	Pa×s	282.10	Joback Method
dvisc	0.0012811	Pa×s	248.94	Joback Method
dvisc	0.0024354	Pa×s	215.78	Joback Method
dvisc	0.0058466	Pa×s	182.62	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52454e+01
Coeff. B	-3.73749e+03
Coeff. C	-5.51300e+01
Temperature range (K), min.	305.00
Temperature range (K), max.	431.37

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=C5187713&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
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

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