2,3-dimethyl-4-pentenal

Inchi: InChI=1S/C7H12O/c1-4-6(2)7(3)5-8/h4-7H,1H2,2-3H3
InchiKey: HXPMOQYQMCGITO-UHFFFAOYSA-N
Formula: C7H12O
SMILES: C=CC(C)C(C)C=O
Mol. weight [g/mol]: 112.17
CAS: ---

Physical Properties

Property code	Value	Unit	Source
af	0.3241		Cheméo Relay (1.0)
gf	-8.50	kJ/mol	Joback Method
hf	-184.34	kJ/mol	Cheméo Relay (1.0)
hfus	7.85	kJ/mol	Joback Method
hvap	44.25	kJ/mol	Cheméo Relay (1.0)
ie	9.39	eV	Cheméo Relay (1.0)
log10ws	-1.45		Cheméo Relay (1.0)
logp	1.643		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
tb	394.31	K	Cheméo Relay (1.0)
tc	581.36	K	Cheméo Relay (1.0)
tf	226.83	K	Cheméo Relay (1.0)
vc	0.375	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.96	J/mol×K	404.02	Joback Method
cpg	213.06	J/mol×K	434.61	Joback Method
cpg	223.65	J/mol×K	465.20	Joback Method
cpg	233.76	J/mol×K	495.78	Joback Method
cpg	243.40	J/mol×K	526.37	Joback Method
cpg	252.58	J/mol×K	556.96	Joback Method
cpg	261.33	J/mol×K	587.55	Joback Method

dvisc	0.0112802	Pa×s	178.89	Joback Method
dvisc	0.0036201	Pa×s	216.41	Joback Method
dvisc	0.0016255	Pa×s	253.93	Joback Method
dvisc	0.0008970	Pa×s	291.45	Joback Method
dvisc	0.0005669	Pa×s	328.98	Joback Method
dvisc	0.0003935	Pa×s	366.50	Joback Method
dvisc	0.0002924	Pa×s	404.02	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

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method: https://en.wikipedia.org/wiki/Joback_method
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):

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