2,6-dimethyl-2-heptenal

Inchi: InChI=1S/C9H16O/c1-8(2)5-4-6-9(3)7-10/h6-8H,4-5H2,1-3H3/b9-6+
InchiKey: YXVDCUSVRUNXEM-RMKNXTFCSA-N
Formula: C9H16O
SMILES: CC(C=O)=CCCC(C)C
Mol. weight [g/mol]: 140.22
CAS: ---

Physical Properties

Property code	Value	Unit	Source
gf	-5.39	kJ/mol	Joback Method
hf	-212.52	kJ/mol	Joback Method
hfus	16.72	kJ/mol	Joback Method
hvap	42.00	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.568		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	1020.00		NIST Webbook
tb	457.58	K	Joback Method
tc	642.53	K	Joback Method
tf	199.15	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.58	J/mol×K	457.58	Joback Method
cpg	296.03	J/mol×K	488.40	Joback Method
cpg	308.83	J/mol×K	519.23	Joback Method
cpg	321.02	J/mol×K	550.05	Joback Method
cpg	332.61	J/mol×K	580.88	Joback Method
cpg	343.63	J/mol×K	611.70	Joback Method
cpg	354.11	J/mol×K	642.53	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32166e+01
Coeff. B	-3.54204e+03
Coeff. C	-6.79600e+01
Temperature range (K), min.	341.92
Temperature range (K), max.	516.03

Sources

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=R145327&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

Legend

cpg: Ideal gas heat capacity

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

tb: Normal Boiling Point Temperature

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