6-Octenal, 3,7-dimethyl-, (R)-

Other names:	(3R)-(+)-Citronellal
	(R)-(+)-Citronellal
	(R)-3,7-Dimethyloct-6-enal
	3,7-Dimethyl-6-octenal, (3R)-
Inchi:	InChI=1S/C10H18O/c1-9(2)5-4-6-10(3)7-8-11/h5,8,10H,4,6-7H2,1-3H3/t10-/m0/s1
InchiKey:	NEHNMFOYXAPHSD-JTQLQIEISA-N
Formula:	C10H18O
SMILES:	CC(C)=CCCC(C)CC=O
Mol. weight [g/mol]:	154.25
CAS:	2385-77-5

Physical Properties

Property code	Value	Unit	Source
gf	3.03	kJ/mol	Joback Method
hf	-233.16	kJ/mol	Joback Method
hfus	19.31	kJ/mol	Joback Method
hvap	44.22	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.958		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1152.00		NIST Webbook
tb	481.00	K	NIST Webbook
tc	663.60	K	Joback Method
tf	210.42	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.12	J/mol×K	480.46	Joback Method
cpg	340.49	J/mol×K	510.98	Joback Method
cpg	354.17	J/mol×K	541.51	Joback Method
cpg	367.20	J/mol×K	572.03	Joback Method

cpg	379.60	J/mol×K	602.55	Joback Method
cpg	391.40	J/mol×K	633.07	Joback Method
cpg	402.62	J/mol×K	663.60	Joback Method
hvapt	54.90	kJ/mol	310.50	NIST Webbook
hvapt	53.20	kJ/mol	398.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50076e+01
Coeff. B	-4.22056e+03
Coeff. C	-7.47570e+01
Temperature range (K), min.	361.48
Temperature range (K), max.	510.04

Sources

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

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=C2385775&Units=SI

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

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

hvapt: Enthalpy of vaporization at a given temperature

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