7-Octenal, 3,7-dimethyl-

Other names:	Rhodinal
	3,7-Dimethyl-7-octenal
	«alpha»-Citronellal
	3,7-dimethyloct-7-enal
Inchi:	InChI=1S/C10H18O/c1-9(2)5-4-6-10(3)7-8-11/h8,10H,1,4-7H2,2-3H3
InchiKey:	KQZAHMIZMBERJX-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	C=C(C)CCCC(C)CC=O
Mol. weight [g/mol]:	154.25
CAS:	141-26-4

Physical Properties

Property code	Value	Unit	Source
gf	10.65	kJ/mol	Joback Method
hf	-224.95	kJ/mol	Joback Method
hfus	17.83	kJ/mol	Joback Method
hvap	43.60	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.958		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
ripol	1581.00		NIST Webbook
tb	472.98	K	Joback Method
tc	651.52	K	Joback Method
tf	213.74	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.21	J/mol×K	472.98	Joback Method
cpg	339.33	J/mol×K	502.74	Joback Method
cpg	352.82	J/mol×K	532.49	Joback Method
cpg	365.71	J/mol×K	562.25	Joback Method

cpg	378.01	J/mol×K	592.01	Joback Method
cpg	389.74	J/mol×K	621.76	Joback Method
cpg	400.92	J/mol×K	651.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C141264&Units=SI
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

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