Octanal, 3,7-dimethyl-

Other names:	Tetrahydrocitral
	3,7-dimethyloctanal
Inchi:	InChI=1S/C10H20O/c1-9(2)5-4-6-10(3)7-8-11/h8-10H,4-7H2,1-3H3
InchiKey:	UCSIFMPORANABL-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	CC(C)CCCC(C)CC=O
Mol. weight [g/mol]:	156.27
CAS:	5988-91-0

Physical Properties

Property code	Value	Unit	Source
gf	-71.08	kJ/mol	Joback Method
hf	-345.87	kJ/mol	Joback Method
hfus	16.90	kJ/mol	Joback Method
hvap	43.80	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	3.038		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
rinpol	1156.00		NIST Webbook
rinpol	1156.00		NIST Webbook
tb	475.98	K	Joback Method
tc	651.64	K	Joback Method
tf	214.46	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.90	J/mol×K	475.98	Joback Method
cpg	357.72	J/mol×K	505.26	Joback Method
cpg	371.91	J/mol×K	534.53	Joback Method
cpg	385.50	J/mol×K	563.81	Joback Method
cpg	398.50	J/mol×K	593.09	Joback Method

cpg	410.94	J/mol×K	622.37	Joback Method
cpg	422.81	J/mol×K	651.64	Joback Method
dvisc	0.0128629	Pa×s	214.46	Joback Method
dvisc	0.0038843	Pa×s	258.05	Joback Method
dvisc	0.0016580	Pa×s	301.63	Joback Method
dvisc	0.0008774	Pa×s	345.22	Joback Method
dvisc	0.0005355	Pa×s	388.81	Joback Method
dvisc	0.0003611	Pa×s	432.39	Joback Method
dvisc	0.0002617	Pa×s	475.98	Joback Method

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=C5988910&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume