Octanal, 7-hydroxy-3,7-dimethyl-

Other names:	Hydroxycitronellal
	Citronellal hydrate
	Citronellal, hydroxy-
	Cyclalia
	Cyclosia
	Fixol
	Laurine
	Lilyl aldehyde
	Muguet synthetic
	Muguettine principle
	Phixia
	3,7-Dimethyl-7-hydroxyoctanal
	7-Hydroxy-3,7-dimethyloctanal
	7-Hydroxycitronellal
	Musuet synthetic
	Musuettine principle
	1-Octanal, 3,7-dimethyl-7-hydroxy-
	7-Hydroxy-3,7-dimethyloctan-1-al
	NSC 406740
Inchi:	InChI=1S/C10H20O2/c1-9(6-8-11)5-4-7-10(2,3)12/h8-9,12H,4-7H2,1-3H3
InchiKey:	WPFVBOQKRVRMJB-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CC(CC=O)CCCC(C)(C)O
Mol. weight [g/mol]:	172.26
CAS:	107-75-5

Physical Properties

Property code	Value	Unit	Source
gf	-202.62	kJ/mol	Joback Method
hf	-501.57	kJ/mol	Joback Method
hfus	17.10	kJ/mol	Joback Method
hvap	75.30	kJ/mol	NIST Webbook
log10ws	-2.42		Crippen Method
logp	2.153		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1269.00		NIST Webbook

rinpol	1269.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1255.20		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1240.60		NIST Webbook
rinpol	1242.50		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1255.20		NIST Webbook
ripol	1882.00		NIST Webbook
ripol	1942.40		NIST Webbook
ripol	1944.20		NIST Webbook
ripol	1915.00		NIST Webbook
ripol	1944.20		NIST Webbook
ripol	1947.00		NIST Webbook
ripol	1882.00		NIST Webbook
ripol	1915.00		NIST Webbook
ripol	1882.00		NIST Webbook
tb	565.37	K	Joback Method
tc	739.88	K	Joback Method
tf	292.70	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.96	J/mol×K	565.37	Joback Method
cpg	420.03	J/mol×K	594.46	Joback Method

cpg	432.44	J/mol×K	623.54	Joback Method
cpg	444.23	J/mol×K	652.63	Joback Method
cpg	455.42	J/mol×K	681.71	Joback Method
cpg	466.05	J/mol×K	710.80	Joback Method
cpg	476.13	J/mol×K	739.88	Joback Method
dvisc	0.0295891	Pa×s	292.70	Joback Method
dvisc	0.0060903	Pa×s	338.14	Joback Method
dvisc	0.0018231	Pa×s	383.59	Joback Method
dvisc	0.0007046	Pa×s	429.03	Joback Method
dvisc	0.0003267	Pa×s	474.48	Joback Method
dvisc	0.0001733	Pa×s	519.92	Joback Method
dvisc	0.0001018	Pa×s	565.37	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C107755&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

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

vc: Critical Volume