2,6-Octadienal, 3,7-dimethyl-, (E)-

Other names:	«alpha»-Citral
	(E)-Citral
	trans-Citral
	trans-3,7-Dimethyl-2,6-octadienal
	Citral a
	Geranaldehyde
	Geranial
	Citral «alpha»
	(E)-3,7-Dimethyl-2,6-octadienal
	(E)-3,7-Dimethylocta-2,6-dienal
	trans-3,7-dimethyl-octa-2,6-dienal
	(E)-Geranial
	(E)-Neral
	2,6-Octadienal, 3,7-dimethyl-, (2E)-
	«beta»-Geranial
	trans-3,7-dimethyl-2,6-octadienal (geranial)
	E-Citral (geranial)
	geranial («alpha»-Citral)
Inchi:	InChI=1S/C10H16O/c1-9(2)5-4-6-10(3)7-8-11/h5,7-8H,4,6H2,1-3H3/b10-7+
InchiKey:	WTEVQBCEXWBHNA-JXMROGBWSA-N
Formula:	C10H16O
SMILES:	CC(C)=CCCC(C)=CC=O
Mol. weight [g/mol]:	152.23
CAS:	141-27-5

Physical Properties

Property code	Value	Unit	Source
gf	77.14	kJ/mol	Joback Method
hf	-120.45	kJ/mol	Joback Method
hfus	21.73	kJ/mol	Joback Method
hvap	62.50	kJ/mol	NIST Webbook
hvap	61.00	kJ/mol	NIST Webbook
log10ws	-3.00		Crippen Method
logp	2.878		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	1271.00		NIST Webbook

rinpol	1269.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1277.00	NIST Webbook
rinpol	1269.00	NIST Webbook
rinpol	1268.00	NIST Webbook
rinpol	1275.00	NIST Webbook
rinpol	1269.00	NIST Webbook
rinpol	1271.00	NIST Webbook
rinpol	1279.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1273.00	NIST Webbook
rinpol	1241.00	NIST Webbook
rinpol	1268.00	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1218.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1236.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1260.00	NIST Webbook
rinpol	1223.00	NIST Webbook
rinpol	1268.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1268.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1275.00	NIST Webbook
rinpol	1268.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1271.00	NIST Webbook
rinpol	1271.00	NIST Webbook
rinpol	1275.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1241.00	NIST Webbook
rinpol	1262.00	NIST Webbook
rinpol	1265.00	NIST Webbook
rinpol	1264.00	NIST Webbook

rinpol	1287.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1278.00		NIST Webbook
ripol	1743.00		NIST Webbook
ripol	1735.00		NIST Webbook
ripol	1733.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1731.00		NIST Webbook
ripol	1718.00		NIST Webbook
ripol	1729.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1730.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1721.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1726.00		NIST Webbook
ripol	1738.00		NIST Webbook
tb	502.20	K	NIST Webbook
tc	675.98	K	Joback Method
tf	206.38	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.04	J/mol×K	484.94	Joback Method
cpg	322.90	J/mol×K	516.78	Joback Method
cpg	336.01	J/mol×K	548.62	Joback Method
cpg	348.41	J/mol×K	580.46	Joback Method
cpg	360.14	J/mol×K	612.30	Joback Method
cpg	371.25	J/mol×K	644.14	Joback Method
cpg	381.76	J/mol×K	675.98	Joback Method
hvapt	54.90	kJ/mol	437.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	391.70	K	2.70	NIST Webbook

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=C141275&Units=SI
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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume