

# 6-Octen-1-ol, 3,7-dimethyl-, (R)-

<b>Other names:</b>	(-)-beta-citronellol (-)-citronellol (R)-(+)«beta»-Citronellol (R)-3,7-dimethyloct-6-en-1-ol (R)-citronellol (S)-(-)-B-citronellol (S)-(-)-citronellol (S)-3,7-dimethyl-6-octen-1-ol L-citronellol
<b>Inchi:</b>	InChI=1S/C10H20O/c1-9(2)5-4-6-10(3)7-8-11/h5,10-11H,4,6-8H2,1-3H3/t10-/m0/s1
<b>InchiKey:</b>	QMVPMAAFGQKVCJ-JTQLQIEISA-N
<b>Formula:</b>	C10H20O
<b>SMILES:</b>	CC(C)=CCCC(C)CCO
<b>Mol. weight [g/mol]:</b>	156.27
<b>CAS:</b>	1117-61-9

## Physical Properties

Property code	Value	Unit	Source
gf	-34.27	kJ/mol	Joback Method
hf	-299.81	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	54.18	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.751		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	1220.00		NIST Webbook
rinpol	1220.00		NIST Webbook
tb	523.98	K	Joback Method
tc	694.42	K	Joback Method
tf	229.24	K	Joback Method
vc	0.590	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.91	J/mol×K	523.98	Joback Method
cpg	376.24	J/mol×K	552.39	Joback Method
cpg	388.99	J/mol×K	580.79	Joback Method
cpg	401.17	J/mol×K	609.20	Joback Method
cpg	412.81	J/mol×K	637.61	Joback Method
cpg	423.93	J/mol×K	666.01	Joback Method
cpg	434.56	J/mol×K	694.42	Joback Method
pvap	1.33e-03	kPa	293.17	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	1.33e-03	kPa	293.17	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	1.32e-03	kPa	293.17	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	2.27e-03	kPa	298.18	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	2.27e-03	kPa	298.19	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	2.27e-03	kPa	298.20	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	3.79e-03	kPa	303.16	Vapor pressures and thermophysical properties of selected monoterpenoids

pvap	3.81e-03	kPa	303.19	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	3.80e-03	kPa	303.20	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	6.21e-03	kPa	308.19	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	6.20e-03	kPa	308.19	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	6.20e-03	kPa	308.21	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	9.90e-03	kPa	313.20	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	9.90e-03	kPa	313.21	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	9.91e-03	kPa	313.21	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.02	kPa	318.23	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.02	kPa	318.24	Vapor pressures and thermophysical properties of selected monoterpenoids

pvap	0.02	kPa	318.24	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.02	kPa	323.22	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.02	kPa	323.23	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.02	kPa	323.23	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.04	kPa	328.20	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.04	kPa	328.21	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.04	kPa	328.21	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.06	kPa	333.23	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.06	kPa	333.23	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.06	kPa	333.23	Vapor pressures and thermophysical properties of selected monoterpenoids

pvap	0.08	kPa	338.19	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.08	kPa	338.20	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.08	kPa	338.20	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.12	kPa	343.19	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.12	kPa	343.19	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.12	kPa	343.19	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.17	kPa	348.14	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.17	kPa	348.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.17	kPa	348.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.24	kPa	353.10	Vapor pressures and thermophysical properties of selected monoterpenoids

pvap	0.24	kPa	353.10	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.24	kPa	353.10	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.33	kPa	358.01	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.33	kPa	358.02	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.33	kPa	358.02	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.46	kPa	362.97	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.46	kPa	362.98	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	0.46	kPa	362.98	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	1.29e-04	kPa	273.65	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	1.30e-04	kPa	273.65	Vapor pressures and thermophysical properties of selected monoterpenoids

pvap	1.33e-04	kPa	273.65	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	2.31e-04	kPa	278.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	2.28e-04	kPa	278.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	2.35e-04	kPa	278.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	4.30e-04	kPa	283.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	4.32e-04	kPa	283.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	4.30e-04	kPa	283.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	7.70e-04	kPa	288.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	7.77e-04	kPa	288.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	7.79e-04	kPa	288.15	Vapor pressures and thermophysical properties of selected monoterpenoids

pvap	1.36e-03	kPa	293.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	1.36e-03	kPa	293.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	1.36e-03	kPa	293.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	2.33e-03	kPa	298.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	2.33e-03	kPa	298.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	2.32e-03	kPa	298.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	3.87e-03	kPa	303.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	3.87e-03	kPa	303.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	3.88e-03	kPa	303.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	6.28e-03	kPa	308.15	Vapor pressures and thermophysical properties of selected monoterpenoids

pvap	6.30e-03	kPa	308.15	Vapor pressures and thermophysical properties of selected monoterpenoids
pvap	6.30e-03	kPa	308.15	Vapor pressures and thermophysical properties of selected monoterpenoids

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	385.70	K	1.60	NIST Webbook

## Sources

**Vapor pressures and thermophysical properties of selected monoterpenoids:** <https://www.doi.org/10.1016/j.fluid.2015.07.031>  
**Joback Method:** [https://en.wikipedia.org/wiki/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=C1117619&Units=SI>

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

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure

<b>rinp0l:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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