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

Other names:	(-)-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
Inchi:	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
InchiKey:	QMVPMAAFGQKVCJ-JTQLQIEISA-N
Formula:	C10H20O
SMILES:	CC(C)=CCCC(C)CCO
Mol. weight [g/mol]:	156.27
CAS:	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

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1117619&Units=SI

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
pvap: Vapor pressure

rinpol:	Non-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