

1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)-

Other names:	(.+-.)-trans-nerolidol (.+/-.)-trans-Nerolidol (6E)-3,7,11-trimethyl-1,6,10-dodecatrien-3-ol (6E)-Nerolidol (E)-3,7,11-trimethyldodeca-1,6,10-trien-3-ol (E)-nerolidol 1-geranyl-2-methyl-3-buten-2-ol 3,7,11-Trimethyl-1,6,10-dodecatrien-3-ol, (E)- E-Nerolidol Nerolidol, E- Nerolidol, trans Trans-(E)-Nerolidol trans-3,7,11-Trimethyl-dodeca-1,6,10-trien-3-ol trans-Nerolidol trans-«beta»-Nerolidol
Inchi:	InChI=1S/C15H26O/c1-6-15(5,16)12-8-11-14(4)10-7-9-13(2)3/h6,9,11,16H,1,7-8,10,12H
InchiKey:	FQTLCLSUCSAZDY-SDNWHVSQSA-N
Formula:	C15H26O
SMILES:	C=CC(C)(O)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	222.37
CAS:	40716-66-3

Physical Properties

Property code	Value	Unit	Source
gf	172.62	kJ/mol	Joback Method
hf	-173.62	kJ/mol	Joback Method
hfus	27.78	kJ/mol	Joback Method
hvap	63.77	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.396		Crippen Method
mcvol	215.180	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
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ripol	2033.00	NIST Webbook
ripol	2046.00	NIST Webbook
ripol	2051.00	NIST Webbook
ripol	2052.00	NIST Webbook
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ripol	2054.00	NIST Webbook
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ripol	2035.00	NIST Webbook
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ripol	2042.00	NIST Webbook

ripol	2076.00		NIST Webbook
ripol	2043.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2055.00		NIST Webbook
ripol	2052.00		NIST Webbook
tb	636.31	K	Joback Method
tc	817.59	K	Joback Method
tf	282.21	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.19	J/mol×K	636.31	Joback Method
cpg	591.00	J/mol×K	666.52	Joback Method
cpg	605.97	J/mol×K	696.74	Joback Method
cpg	620.16	J/mol×K	726.95	Joback Method
cpg	633.63	J/mol×K	757.17	Joback Method
cpg	646.44	J/mol×K	787.38	Joback Method
cpg	658.66	J/mol×K	817.59	Joback Method
hvapt	92.70	kJ/mol	298.00	Evaluation of vaporization enthalpies and liquid vapor pressures of cedrol, nerolidol, and 1-adamantanol by correlation gas chromatography

Sources

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Evaluation of vaporization enthalpies and liquid vapor pressures of cedrol, nerolidol, and 1-adamantanol by correlation gas chromatography:
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https://en.wikipedia.org/wiki/Joback_method

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<http://webbook.nist.gov/cgi/cbook.cgi?ID=C40716663&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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