Nerolidol

Other names:	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, [S-(Z)]-
	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (Z)-(S)-(+)-
	(+)-Nerolidol
	D-Nerolidol
	Nerolidol, cis-(+)-
	Peruviol
	3,7,11-Trimethyl-1,6,10-dodecatriene-3-ol, (Z)-(S)-(+)-
	(6Z)-3,7,11-Trimethyl-1,6,10-dodecatrien-3-ol
	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (3S,6Z)-
	NSC 60598
	(Z)-Nerolidol
	cis-Nerolidol
	Nerolidol (Z)
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-KAMYIIQDSA-N
Formula:	C15H26O
SMILES:	C=CC(C)(O)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	222.37
CAS:	142-50-7

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
rinpol	1535.00		NIST Webbook
rinpol	1554.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1531.00		NIST Webbook

rinpol	1546.00	NIST Webbook
rinpol	1522.00	NIST Webbook
rinpol	1522.00	NIST Webbook
rinpol	1504.00	NIST Webbook
rinpol	1543.00	NIST Webbook
rinpol	1565.00	NIST Webbook
rinpol	1509.00	NIST Webbook
rinpol	1534.00	NIST Webbook
rinpol	1526.00	NIST Webbook
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rinpol	1501.00	NIST Webbook
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rinpol	1534.00	NIST Webbook
rinpol	1541.00	NIST Webbook
rinpol	1535.00	NIST Webbook
rinpol	1534.00	NIST Webbook
ripol	2023.00	NIST Webbook
ripol	2008.00	NIST Webbook
ripol	2027.00	NIST Webbook
ripol	1984.00	NIST Webbook
ripol	2008.00	NIST Webbook
ripol	2005.00	NIST Webbook
ripol	2010.00	NIST Webbook
ripol	2011.00	NIST Webbook
ripol	2008.00	NIST Webbook
ripol	1984.00	NIST Webbook
ripol	2023.00	NIST Webbook
ripol	2018.00	NIST Webbook
ripol	1993.00	NIST Webbook
ripol	2031.00	NIST Webbook
ripol	1992.00	NIST Webbook
ripol	1994.00	NIST Webbook
ripol	1961.00	NIST Webbook
ripol	2005.00	NIST Webbook
ripol	2005.00	NIST Webbook
ripol	2014.00	NIST Webbook
ripol	1997.00	NIST Webbook
ripol	2034.00	NIST Webbook
ripol	1995.00	NIST Webbook

ripol	2039.00		NIST Webbook
ripol	2006.00		NIST Webbook
ripol	2009.00		NIST Webbook
ripol	2018.00		NIST Webbook
tb	549.20	K	NIST Webbook
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

Sources

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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

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
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