

2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)-

Other names:	(2Z)-3,7-Dimethyl-2,6-octadien-1-ol (Z)-3,7-Dimethyl-2,6-octadien-1-ol (Z)-Geraniol (Z)-Nerol 2,6-Dimethyl-2,6-octadien-8-ol 2,6-Octadien-1-ol, 3,7-dimethyl-, (2Z)- 2-cis-3,7-Dimethyl-2,6-octadien-1-ol 3,7-Dimethyl-2,6-octadien-1-ol 3,7-Dimethyl-2,6-octadien-1-ol, cis- Nerol Nerol (cis-geraniol) Neryl alcohol Vernol cis-2,6-Dimethyl-2,6-octadien-8-ol cis-3,7-Dimethyl-2,6-octadien-1-ol cis-Geraniol
Inchi:	InChI=1S/C10H18O/c1-9(2)5-4-6-10(3)7-8-11/h5,7,11H,4,6,8H2,1-3H3/b10-7-
InchiKey:	GLZPCOQZEFWAFX-YFHOOEESVSA-N
Formula:	C10H18O
SMILES:	CC(C)=CCCC(C)=CCO
Mol. weight [g/mol]:	154.25
CAS:	106-25-2

Physical Properties

Property code	Value	Unit	Source
gf	39.84	kJ/mol	Joback Method
hf	-187.10	kJ/mol	Joback Method
hfus	23.53	kJ/mol	Joback Method
hvap	54.61	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.671		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
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ripol	1790.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1808.00		NIST Webbook
ripol	1808.00		NIST Webbook
ripol	1808.00		NIST Webbook
ripol	1790.00		NIST Webbook
ripol	1808.00		NIST Webbook
ripol	1839.00		NIST Webbook
ripol	1788.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1808.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1808.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1794.00		NIST Webbook
ripol	1802.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1786.00		NIST Webbook
ripol	1821.00		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1810.00		NIST Webbook
ripol	1757.00		NIST Webbook
ripol	1781.00		NIST Webbook
ripol	1790.00		NIST Webbook
ripol	1808.00		NIST Webbook
ripol	1782.00		NIST Webbook
tb	528.46	K	Joback Method

tc	705.46	K	Joback Method
tf	225.20	K	Joback Method
vc	0.577	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.44	J/mol×K	528.46	Joback Method
cpg	357.23	J/mol×K	557.96	Joback Method
cpg	369.40	J/mol×K	587.46	Joback Method
cpg	380.97	J/mol×K	616.96	Joback Method
cpg	391.97	J/mol×K	646.46	Joback Method
cpg	402.45	J/mol×K	675.96	Joback Method
cpg	412.43	J/mol×K	705.46	Joback Method
hvapt	55.40	kJ/mol	416.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	377.20	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57087e+01
Coeff. B	-4.67082e+03
Coeff. C	-7.96360e+01
Temperature range (K), min.	382.52
Temperature range (K), max.	528.87

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C106252&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
pvap:	Vapor 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

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