

Nerol oxide

Other names:	2H-Pyran, 3,6-dihydro-4-methyl-2-(2-methyl-1-propen-1-yl)- 3,6-Dihydro-4-methyl-2-(2-methyl-1-propenyl)-2H-pyran Isoneroloxide Nerol oxide Neryl oxide
Inchi:	InChI=1S/C10H16O/c1-8(2)6-10-7-9(3)4-5-11-10/h4,6,10H,5,7H2,1-3H3
InchiKey:	FRISMOQHRTLZZRP-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC(C)=CC1CC(C)=CCO1
Mol. weight [g/mol]:	152.24

Physical Properties

Property code	Value	Unit	Source
hfus	21.19	kJ/mol	Joback Method
logp	2.688		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
rinpol	1144.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1140.00		NIST Webbook

rinpol	1163.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1155.00	NIST Webbook
rinpol	1155.20	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1138.00	NIST Webbook
rinpol	1153.00	NIST Webbook
rinpol	1138.00	NIST Webbook
rinpol	1138.00	NIST Webbook
rinpol	1164.00	NIST Webbook
rinpol	1137.00	NIST Webbook
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rinpol	1147.00	NIST Webbook
rinpol	1151.00	NIST Webbook
rinpol	1172.00	NIST Webbook
ripol	1480.00	NIST Webbook
ripol	1469.00	NIST Webbook
ripol	1466.00	NIST Webbook
ripol	1469.00	NIST Webbook
ripol	1460.00	NIST Webbook
ripol	1471.00	NIST Webbook
ripol	1466.00	NIST Webbook
ripol	1469.00	NIST Webbook
ripol	1480.00	NIST Webbook
ripol	1478.00	NIST Webbook
ripol	1450.00	NIST Webbook
ripol	1489.00	NIST Webbook
ripol	1481.00	NIST Webbook
ripol	1480.00	NIST Webbook
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ripol	1473.00	NIST Webbook
ripol	1464.00	NIST Webbook
ripol	1468.00	NIST Webbook
ripol	1450.00	NIST Webbook
ripol	1463.00	NIST Webbook
ripol	1450.00	NIST Webbook
ripol	1471.00	NIST Webbook
ripol	1465.00	NIST Webbook
ripol	1468.50	NIST Webbook
ripol	1466.00	NIST Webbook
ripol	1500.00	NIST Webbook
ripol	1466.00	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.69	J/mol×K	482.88	Joback Method
cpg	319.98	J/mol×K	518.44	Joback Method
cpg	336.31	J/mol×K	554.01	Joback Method
cpg	351.71	J/mol×K	589.57	Joback Method
cpg	366.23	J/mol×K	625.13	Joback Method
cpg	379.89	J/mol×K	660.70	Joback Method
cpg	392.74	J/mol×K	696.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1786089&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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