

2H-Pyran-3-ol, 6-ethenyltetrahydro-2,2,6-trimethyl-

Other names:	2H-Pyran-3-ol, tetrahydro-2,2,6-trimethyl-6-vinyl-Epoxyllinalol 3-Hydroxy-2,2,6-trimethyl-6-vinyltetrahydropyran 2,2,6-Trimethyl-6-vinyltetrahydro-2H-pyran-3-ol 2,6,6-trimethyl-2-vinyl-5-hydroxytetrahydropyran Linalool oxide Linalool oxide (pyranoid) Linalool oxide pyranoside linalool oxide C (2,6,6-trimethyl-2-vinyl-5-hydroxytetrahydropyran) tetrahydro-2,2,6-trimethyl-6-vinyl-2H-pyran-3-ol
Inchi:	InChI=1S/C10H18O2/c1-5-10(4)7-6-8(11)9(2,3)12-10/h5,8,11H,1,6-7H2,2-4H3
InchiKey:	BCTBAGTXFYWYMW-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	C=CC1(C)CCC(O)C(C)(C)O1
Mol. weight [g/mol]:	170.25
CAS:	14049-11-7

Physical Properties

Property code	Value	Unit	Source
gf	-103.73	kJ/mol	Joback Method
hf	-364.41	kJ/mol	Joback Method
hfus	13.82	kJ/mol	Joback Method
hvap	55.88	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.881		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1198.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1136.00		NIST Webbook
ripol	1720.00		NIST Webbook

ripol	1721.00		NIST Webbook
tb	554.70	K	Joback Method
tc	757.96	K	Joback Method
tf	334.79	K	Joback Method
vc	0.543	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.60	J/mol×K	554.70	Joback Method
cpg	397.07	J/mol×K	588.58	Joback Method
cpg	411.62	J/mol×K	622.45	Joback Method
cpg	425.40	J/mol×K	656.33	Joback Method
cpg	438.57	J/mol×K	690.21	Joback Method
cpg	451.29	J/mol×K	724.08	Joback Method
cpg	463.72	J/mol×K	757.96	Joback Method

Sources

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=C14049117&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
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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