

(3R,6R)-2,2,6-Trimethyl-6-vinyltetrahydro-2H-pyra

Other names:

cis-Linalool 3,7-oxide
cis-Pyranoid linalool oxide
Linalool 3,7-oxide, cis-
Pyranoid linalool oxide, cis-
cis-Linalool Oxide, pyranoid
linalool oxide, cis-pyranoid
cis-linalool pyran oxide
(Z)-Linalol pyranoxide
cis-Linalool oxide (pyran)
(Z)-pyran linalool oxide
cis-pyran linalool oxide
cis-Linalol oxide (pyranoid)
(Z)-linalool oxide (pyranoid)
cis-Linalool oxide (pyranyl ring)
cis-2,6-Dimethyl-2,6-epoxy-7-octen-3-ol
cis-linalol pyranoxide
cis-pyranic linalool oxid
linalool oxide III (cis, pyranoid)
Z-Pyranoid linalool oxide
Linalool oxide (pyranoid) cis
cis-linalool pyranoid oxide
(Z)-Linallol oxide (pyran)

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/t8-,10+/m
InchiKey: BCTBAGTXFYWYMW-SCZZXKLOSA-N
Formula: C10H18O2
SMILES: C=CC1(C)CCC(O)C(C)(C)O1
Mol. weight [g/mol]: 170.25
CAS: 14009-71-3

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	1157.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1167.00		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1746.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1763.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1724.00		NIST Webbook
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ripol	1743.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1754.00		NIST Webbook
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ripol	1772.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1739.00		NIST Webbook
ripol	1763.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1708.00		NIST Webbook
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ripol	1769.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1758.00		NIST Webbook
ripol	1708.00		NIST Webbook
ripol	1768.80		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1742.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1758.00		NIST Webbook
ripol	1708.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1770.00		NIST Webbook
ripol	1768.00		NIST Webbook
ripol	1770.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1718.00		NIST Webbook
ripol	1742.00		NIST Webbook
ripol	1763.00		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/molxK	554.70	Joback Method
cpg	397.07	J/molxK	588.58	Joback Method
cpg	411.62	J/molxK	622.45	Joback Method
cpg	425.40	J/molxK	656.33	Joback Method
cpg	438.57	J/molxK	690.21	Joback Method
cpg	451.29	J/molxK	724.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14009713&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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