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

Other names: trans-Linalool 3,7-oxide
trans-Pyranoid linalool oxide
Linalool 3,7-oxide, trans-
Pyranoid linalool oxide, trans-
trans-linalool oxide (pyranoid)
linalool oxide, trans-pyranoid
(E)-pyran linalool oxide
(E)-Linalool oxide (pyranoid)
(E)-Linalol pyranoxide
trans-Linalool oxide (pyran)
trans-Linalol oxide (pyranoid)
Linalool oxide I (pyran)
trans-pyran linalool oxide
linalool oxide C (trans-THP)
trans-Linalool oxide (pyranyl ring)
linalool oxide (III)
t-Pyran linalool oxide
Linalool oxide I (pyranoid)
trans-pyranic linalool oxide
trans-pyranic linalool oxid
(E)-Linallol oxide (pyran)
E-Pyranoid linalool oxide
linalool oxide IV (trans, pyranoid)
Linalool E-pyranic oxide

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: 39028-58-5

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	1169.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1199.00		NIST Webbook
ripol	1759.00		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1753.00		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1729.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1698.00		NIST Webbook
ripol	1698.00		NIST Webbook
ripol	1749.00		NIST Webbook
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ripol	1736.00		NIST Webbook
ripol	1735.00		NIST Webbook

ripol	1732.00		NIST Webbook
ripol	1770.00		NIST Webbook
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ripol	1755.00		NIST Webbook
ripol	1716.00		NIST Webbook
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ripol	1716.00		NIST Webbook
ripol	1731.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1719.00		NIST Webbook
ripol	1746.00		NIST Webbook
ripol	1724.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1739.00		NIST Webbook
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ripol	1742.30		NIST Webbook
ripol	1770.00		NIST Webbook
ripol	1717.00		NIST Webbook
ripol	1731.00		NIST Webbook
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ripol	1740.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1722.00		NIST Webbook
ripol	1716.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1778.00		NIST Webbook
ripol	1727.00		NIST Webbook
ripol	1724.00		NIST Webbook
tb	554.70	K	Joback Method
tc	757.96	K	Joback Method
tf	334.79	K	Joback Method
vc	0.543	m3/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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C39028585&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

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