

cis-Linaloloxide

Other names:	cis-Linalol oxide (furanoid) cis-Linalol oxide (f) cis-Linalol oxide fur. (Z)-Linalol oxide
Inchi:	InChI=1S/C10H18O2/c1-5-10(4,11)7-6-8-9(2,3)12-8/h5,8,11H,1,6-7H2,2-4H3
InchiKey:	SATQWIIUJKWZNO-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	C=CC(C)(O)CCC1OC1(C)C
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
gf	-51.39	kJ/mol	Joback Method
hf	-349.58	kJ/mol	Joback Method
hfus	17.94	kJ/mol	Joback Method
hvap	55.53	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.881		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1069.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1062.00		NIST Webbook

ripol	1057.00		NIST Webbook
ripol	1087.00		NIST Webbook
ripol	1075.00		NIST Webbook
ripol	1435.00		NIST Webbook
ripol	1468.00		NIST Webbook
ripol	1475.00		NIST Webbook
ripol	1479.00		NIST Webbook
ripol	1485.00		NIST Webbook
ripol	1484.00		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1439.00		NIST Webbook
ripol	1485.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1465.00		NIST Webbook
ripol	1444.00		NIST Webbook
tb	543.09	K	Joback Method
tc	730.69	K	Joback Method
tf	328.11	K	Joback Method
vc	0.559	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.52	J/mol×K	543.09	Joback Method
cpg	396.33	J/mol×K	574.36	Joback Method
cpg	409.26	J/mol×K	605.62	Joback Method
cpg	421.41	J/mol×K	636.89	Joback Method
cpg	432.89	J/mol×K	668.16	Joback Method
cpg	443.80	J/mol×K	699.42	Joback Method
cpg	454.24	J/mol×K	730.69	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U121974&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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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