

(+)-(E)-Limonene oxide

Other names:	trans-d--Limonene oxide (+)-trans-Limonene 1,2-epoxide R-(+)-Limonene oxide (+)-trans-limonene oxide
Inchi:	InChI=1S/C10H16O/c1-7(2)8-4-5-10(3)9(6-8)11-10/h8-9H,1,4-6H2,2-3H3/t8-,9?,10-/m0/s
InchiKey:	CCEFMUBVSUDRLG-SMILAEQMSA-N
Formula:	C10H16O
SMILES:	C=C(C)C1CCC2(C)OC2C1
Mol. weight [g/mol]:	152.23
CAS:	6909-30-4

Physical Properties

Property code	Value	Unit	Source
gf	122.69	kJ/mol	Joback Method
hf	-131.75	kJ/mol	Joback Method
hfus	15.99	kJ/mol	Joback Method
hvap	40.31	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.520		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
rinpol	1130.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1139.00		NIST Webbook
ripol	1470.00		NIST Webbook
ripol	1472.00		NIST Webbook
ripol	1470.00		NIST Webbook
tb	465.03	K	Joback Method
tc	678.77	K	Joback Method
tf	265.33	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.56	J/mol×K	465.03	Joback Method
cpg	322.20	J/mol×K	500.65	Joback Method
cpg	339.41	J/mol×K	536.28	Joback Method
cpg	355.33	J/mol×K	571.90	Joback Method
cpg	370.12	J/mol×K	607.52	Joback Method
cpg	383.92	J/mol×K	643.14	Joback Method
cpg	396.88	J/mol×K	678.77	Joback Method

Sources

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=C6909304&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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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