

8,9-Limonene oxide (isomer 1)

Inchi:	InChI=1S/C10H16O/c1-8-3-5-9(6-4-8)10(2)7-11-10/h3,9H,4-7H2,1-2H3
InchiKey:	PJGRMBOWSWHGDV-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC1=CCC(C2(C)CO2)CC1
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	47.24	kJ/mol	Joback Method
hf	-193.06	kJ/mol	Joback Method
hfus	14.14	kJ/mol	Joback Method
hvap	42.51	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.522		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
ripol	1181.00		NIST Webbook
ripol	1535.00		NIST Webbook
ripol	1535.00		NIST Webbook
tb	485.82	K	Joback Method
tc	711.15	K	Joback Method
tf	291.53	K	Joback Method
vc	0.490	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.80	J/mol×K	485.82	Joback Method
cpg	324.55	J/mol×K	523.38	Joback Method
cpg	341.89	J/mol×K	560.93	Joback Method
cpg	357.98	J/mol×K	598.49	Joback Method
cpg	372.97	J/mol×K	636.04	Joback Method
cpg	387.02	J/mol×K	673.60	Joback Method
cpg	400.28	J/mol×K	711.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R601213&Units=SI
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

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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