trans-Ocimene oxide

Inchi: InChI=1S/C9H14O/c1-7(2)5-4-6-9-8(3)10-9/h4-6,8-9H,1-3H3/b6-4+/t8-,9-/m1/s1
InchiKey: OWSPFEVOQIITLR-FVOAXITGSA-N
Formula: C9H14O
SMILES: CC(C)=CC=CC1OC1C
Mol. weight [g/mol]: 138.21

Physical Properties

Property code	Value	Unit	Source
gf	143.71	kJ/mol	Joback Method
hf	-83.98	kJ/mol	Joback Method
hfus	25.35	kJ/mol	Joback Method
hvap	39.74	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.296		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	1141.00		NIST Webbook
rinpol	1141.00		NIST Webbook
tb	442.54	K	Joback Method
tc	641.03	K	Joback Method
tf	207.34	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.17	J/mol×K	442.54	Joback Method
cpg	274.36	J/mol×K	475.62	Joback Method
cpg	288.63	J/mol×K	508.70	Joback Method
cpg	302.02	J/mol×K	541.79	Joback Method
cpg	314.60	J/mol×K	574.87	Joback Method
cpg	326.42	J/mol×K	607.95	Joback Method
cpg	337.54	J/mol×K	641.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R593345&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume