Epoxyneral

Inchi: InChI=1S/C10H16O2/c1-8(6-7-11)4-5-9-10(2,3)12-9/h6-7,9H,4-5H2,1-3H3/b8-6-
InchiKey: VZUZJYDKCIVBDN-VURMDHGXSA-N
Formula: C10H16O2
SMILES: CC(=CC=O)CCC1OC1(C)C
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-33.10	kJ/mol	Joback Method
hf	-292.18	kJ/mol	Joback Method
hfus	23.72	kJ/mol	Joback Method
hvap	47.58	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.089		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1224.00		NIST Webbook
tb	510.16	K	Joback Method
tc	710.14	K	Joback Method
tf	289.59	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.52	J/mol×K	510.16	Joback Method
cpg	358.16	J/mol×K	543.49	Joback Method
cpg	371.81	J/mol×K	576.82	Joback Method
cpg	384.59	J/mol×K	610.15	Joback Method
cpg	396.62	J/mol×K	643.48	Joback Method
cpg	408.01	J/mol×K	676.81	Joback Method
cpg	418.87	J/mol×K	710.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R435091&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume