(E)-«beta»-10,11-Dihydro-10,11-epoxyfarnesene

Inchi: InChI=1S/C15H24O/c1-6-12(2)8-7-9-13(3)10-11-14-15(4,5)16-14/h6,9,14H,1-2,7-8,10-11
InchiKey: VLCSIBCFYWQTOS-UKTHLTGXSA-N
Formula: C15H24O
SMILES: C=CC(=C)CCC=C(C)CCC1OC1(C)C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	275.65	kJ/mol	Joback Method
hf	-68.73	kJ/mol	Joback Method
hfus	30.51	kJ/mol	Joback Method
hvap	50.72	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.413		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
rinpol	1547.00		NIST Webbook
ripol	1927.00		NIST Webbook
tb	569.14	K	Joback Method
tc	763.20	K	Joback Method
tf	286.46	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.31	J/mol×K	569.14	Joback Method
cpg	539.68	J/mol×K	601.48	Joback Method
cpg	557.00	J/mol×K	633.83	Joback Method
cpg	573.39	J/mol×K	666.17	Joback Method
cpg	588.99	J/mol×K	698.51	Joback Method
cpg	603.90	J/mol×K	730.85	Joback Method
cpg	618.26	J/mol×K	763.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R231502&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume