14-Hydroxy-4,5-epoxy-«beta»-caryophyllene («beta»«alpha»)

Other names: 14-Hydroxy-4,5-epoxy- «beta»-caryophyllene («beta»«alpha»-configuration)
Inchi: InChI=1S/C15H24O2/c1-10-4-5-13-15(9-16,17-13)7-6-12-11(10)8-14(12,2)3/h11-13,16H
InchiKey: PUIHQHPNBOICHY-NSOJWWLLSA-N
Formula: C15H24O2
SMILES: C=C1CCC2OC2(CO)CCC2C1CC2(C)C
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	25.11	kJ/mol	Joback Method
hf	-363.20	kJ/mol	Joback Method
hfus	23.17	kJ/mol	Joback Method
hvap	67.67	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.909		Crippen Method
mcvol	197.070	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
ripol	2663.00		NIST Webbook
ripol	2663.00		NIST Webbook
ripol	2663.00		NIST Webbook
ripol	2663.00		NIST Webbook
tb	685.06	K	Joback Method
tc	897.27	K	Joback Method
tf	442.46	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.01	J/mol×K	685.06	Joback Method
cpg	628.78	J/mol×K	720.43	Joback Method
cpg	646.86	J/mol×K	755.80	Joback Method
cpg	664.48	J/mol×K	791.17	Joback Method
cpg	681.90	J/mol×K	826.54	Joback Method

cpg	699.33	J/mol×K	861.90	Joback Method
cpg	717.01	J/mol×K	897.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R336162&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume