12-nor-2,3-Epoxy-ziza-6(13)-ene

Inchi: InChI=1S/C15H22O/c1-9-11-7-12-14(4,16-12)15(11)6-5-10(8-15)13(9,2)3/h10-12H,1,5-8
InchiKey: BPILZBUHCIZTTB-DNQAXRSOSA-N
Formula: C15H22O
SMILES: C=C1C2CC3OC3(C)C23CCC(C3)C1(C)C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	253.49	kJ/mol	Joback Method
hf	-104.45	kJ/mol	Joback Method
hfus	17.21	kJ/mol	Joback Method
hvap	49.23	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.546		Crippen Method
mcvol	180.340	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	1551.00		NIST Webbook
tb	587.05	K	Joback Method
tc	818.53	K	Joback Method
tf	434.04	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.81	J/mol×K	587.05	Joback Method
cpg	539.52	J/mol×K	625.63	Joback Method
cpg	558.76	J/mol×K	664.21	Joback Method
cpg	577.00	J/mol×K	702.79	Joback Method
cpg	594.71	J/mol×K	741.37	Joback Method
cpg	612.37	J/mol×K	779.95	Joback Method
cpg	630.44	J/mol×K	818.53	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R198579&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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