12-nor-2,3-Epoxyziz-6(13)-ene

Inchi: InChI=1S/C14H20O/c1-8-10-6-11-12(15-11)14(10)5-4-9(7-14)13(8,2)3/h9-12H,1,4-7H2,2
InchiKey: YPJCZNJKSBGJEP-XJKRIIPFSA-N
Formula: C14H20O
SMILES: C=C1C2CC3OC3C23CCC(C3)C1(C)C
Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
gf	250.56	kJ/mol	Joback Method
hf	-99.05	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	48.16	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.156		Crippen Method
mcvol	166.250	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	1550.00		NIST Webbook
ripol	2070.00		NIST Webbook
ripol	2070.00		NIST Webbook
tb	563.93	K	Joback Method
tc	790.58	K	Joback Method
tf	398.87	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.30	J/mol×K	563.93	Joback Method
cpg	489.98	J/mol×K	601.70	Joback Method
cpg	509.04	J/mol×K	639.48	Joback Method
cpg	526.84	J/mol×K	677.25	Joback Method
cpg	543.72	J/mol×K	715.03	Joback Method
cpg	560.01	J/mol×K	752.80	Joback Method
cpg	576.05	J/mol×K	790.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R501361&Units=SI

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