

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:	YPJCZCJKSBGJEP-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
rinpola	1550.00		NIST Webbook
ripola	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.30	J/molxK	563.93	Joback Method
cpg	489.98	J/molxK	601.70	Joback Method
cpg	509.04	J/molxK	639.48	Joback Method
cpg	526.84	J/molxK	677.25	Joback Method
cpg	543.72	J/molxK	715.03	Joback Method
cpg	560.01	J/molxK	752.80	Joback Method
cpg	576.05	J/molxK	790.58	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=R501361&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
ri_{npol}:	Non-polar retention indices
ri_{pol}:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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