13-nor-4,5-Epoxyeudesm-6-en-11-one

Inchi: InChI=1S/C14H20O2/c1-10(15)11-5-8-12(2)6-4-7-13(3)14(12,9-11)16-13/h9H,4-8H2,1-3
InchiKey: TWMMRCHAYIOZQQ-ZFXTZCCVSA-N
Formula: C14H20O2
SMILES: CC(=O)C1=CC23OC2(C)CCCC3(C)CC1
Mol. weight [g/mol]: 220.31

Physical Properties

Property code	Value	Unit	Source
gf	13.87	kJ/mol	Joback Method
hf	-278.76	kJ/mol	Joback Method
hfus	13.74	kJ/mol	Joback Method
hvap	55.60	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.014		Crippen Method
mcvol	178.680	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	1663.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1663.00		NIST Webbook
ripol	2370.00		NIST Webbook
ripol	2370.00		NIST Webbook
tb	634.16	K	Joback Method
tc	877.88	K	Joback Method
tf	455.80	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.31	J/mol×K	634.16	Joback Method
cpg	523.54	J/mol×K	674.78	Joback Method
cpg	540.90	J/mol×K	715.40	Joback Method
cpg	557.90	J/mol×K	756.02	Joback Method
cpg	575.04	J/mol×K	796.64	Joback Method

cpg	592.82	J/mol×K	837.26	Joback Method
cpg	611.74	J/mol×K	877.88	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=R198613&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