10-epi-1,12-epoxycadina-3,11-diene

Inchi: InChI=1S/C15H22O/c1-10-6-7-15-12(3)4-5-13(14(15)8-10)11(2)9-16-15/h6,12-14H,2,4-5
InchiKey: UVENIXMYKAFBBY-UHFFFAOYSA-N
Formula: C15H22O
SMILES: C=C1COC23CC=C(C)CC2C1CCC3C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	183.36	kJ/mol	Joback Method
hf	-165.72	kJ/mol	Joback Method
hfus	23.04	kJ/mol	Joback Method
hvap	53.57	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.714		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
rinpol	1587.00		NIST Webbook
rinpol	1587.00		NIST Webbook
tb	605.72	K	Joback Method
tc	837.31	K	Joback Method
tf	371.74	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.93	J/mol×K	605.72	Joback Method
cpg	544.22	J/mol×K	644.32	Joback Method
cpg	565.07	J/mol×K	682.92	Joback Method
cpg	584.67	J/mol×K	721.51	Joback Method
cpg	603.23	J/mol×K	760.11	Joback Method
cpg	620.93	J/mol×K	798.71	Joback Method
cpg	637.96	J/mol×K	837.31	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=R233499&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume