1,11-Epxoycadina-4,9-diene

Other names: 1,11-Epoxycadina-4,9-diene
Inchi: InChI=1S/C15H22O/c1-10-7-8-15-11(2)5-6-12(13(15)9-10)14(3,4)16-15/h5,9,12-13H,6-8
InchiKey: JQNDHAYUYJSOKV-DNOWBOINSA-N
Formula: C15H22O
SMILES: CC1=CC2C3CC=C(C)C2(CC1)OC3(C)C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	157.22	kJ/mol	Joback Method
hf	-182.25	kJ/mol	Joback Method
hfus	20.83	kJ/mol	Joback Method
hvap	53.05	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.857		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	1484.00		NIST Webbook
ripol	1816.00		NIST Webbook
ripol	1816.00		NIST Webbook
tb	606.67	K	Joback Method
tc	840.69	K	Joback Method
tf	398.76	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.90	J/mol×K	606.67	Joback Method
cpg	539.75	J/mol×K	645.67	Joback Method
cpg	559.32	J/mol×K	684.68	Joback Method
cpg	577.94	J/mol×K	723.68	Joback Method
cpg	595.91	J/mol×K	762.68	Joback Method
cpg	613.56	J/mol×K	801.69	Joback Method

cpg	631.20	J/mol×K	840.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229480&Units=SI
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

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