5,11-Epoxycadin-1(10)-en-9-ol

Inchi: InChI=1S/C15H24O2/c1-8-5-6-10-9(2)12(16)7-11-13(10)14(8)17-15(11,3)4/h8,11-14,16H
InchiKey: NCSPYSIQMMAEMW-UHFFFAOYSA-N
Formula: C15H24O2
SMILES: CC1=C2CCC(C)C3OC(C)(C)C(CC1O)C23
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	-19.49	kJ/mol	Joback Method
hf	-448.18	kJ/mol	Joback Method
hfus	32.14	kJ/mol	Joback Method
hvap	69.97	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.907		Crippen Method
mcvol	197.070	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	1742.00		NIST Webbook
ripol	2611.00		NIST Webbook
tb	690.11	K	Joback Method
tc	897.29	K	Joback Method
tf	426.44	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.68	J/mol×K	690.11	Joback Method
cpg	635.54	J/mol×K	724.64	Joback Method
cpg	653.53	J/mol×K	759.17	Joback Method
cpg	670.77	J/mol×K	793.70	Joback Method
cpg	687.41	J/mol×K	828.23	Joback Method
cpg	703.58	J/mol×K	862.76	Joback Method
cpg	719.42	J/mol×K	897.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R228843&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