6,10-epoxybisabol-2-en-12-al

Inchi: InChI=1S/C15H24O2/c1-10-4-6-13-11(2)5-7-14(12(3)9-16)17-15(13)8-10/h4,6,9-15H,5,7
InchiKey: HAICQTPYRLMCFN-AOAHJRJYSA-N
Formula: C15H24O2
SMILES: CC1C=CC2C(C)CCC(C(C)C=O)OC2C1
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	-44.83	kJ/mol	Joback Method
hf	-464.23	kJ/mol	Joback Method
hfus	31.56	kJ/mol	Joback Method
hvap	59.88	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.217		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1658.00		NIST Webbook
rinpol	1658.00		NIST Webbook
tb	637.75	K	Joback Method
tc	856.49	K	Joback Method
tf	318.70	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.44	J/mol×K	637.75	Joback Method
cpg	616.43	J/mol×K	674.21	Joback Method
cpg	637.96	J/mol×K	710.66	Joback Method
cpg	658.06	J/mol×K	747.12	Joback Method
cpg	676.77	J/mol×K	783.58	Joback Method
cpg	694.11	J/mol×K	820.04	Joback Method
cpg	710.14	J/mol×K	856.49	Joback Method
dvisc	0.0037106	Pa×s	318.70	Joback Method

dvisc	0.0020009	Pa×s	371.88	Joback Method
dvisc	0.0012593	Pa×s	425.05	Joback Method
dvisc	0.0008785	Pa×s	478.23	Joback Method
dvisc	0.0006586	Pa×s	531.40	Joback Method
dvisc	0.0005204	Pa×s	584.58	Joback Method
dvisc	0.0004276	Pa×s	637.75	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=R233533&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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