2-(7Z)-Bisaboladien-4-ol

Inchi: InChI=1S/C15H26O/c1-12(2)6-5-7-13(3)14-8-10-15(4,16)11-9-14/h5-6,8,10,12-14,16H,7,
InchiKey: VPQVBGZEPDUZFM-WAYWQWQTSA-N
Formula: C15H26O
SMILES: CC(C)C=CCC(C)C1C=CC(C)(O)CC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	55.15	kJ/mol	Joback Method
hf	-291.50	kJ/mol	Joback Method
hfus	19.68	kJ/mol	Joback Method
hvap	64.11	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.942		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	1619.00		NIST Webbook
rinpol	1619.00		NIST Webbook
tb	652.34	K	Joback Method
tc	849.78	K	Joback Method
tf	312.35	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.62	J/mol×K	652.34	Joback Method
cpg	604.92	J/mol×K	685.25	Joback Method
cpg	622.32	J/mol×K	718.15	Joback Method
cpg	638.93	J/mol×K	751.06	Joback Method
cpg	654.86	J/mol×K	783.97	Joback Method
cpg	670.21	J/mol×K	816.88	Joback Method
cpg	685.09	J/mol×K	849.78	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=R633344&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