(Z)-Bisabol-11-ol

Inchi: InChI=1S/C15H26O/c1-12-7-9-14(10-8-12)13(2)6-5-11-15(3,4)16/h6-7,14,16H,5,8-11H2,
InchiKey: AXLLSNSRONSXGV-MLPAPPSSSA-N
Formula: C15H26O
SMILES: CC1=CCC(C(C)=CCCC(C)(C)O)CC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	57.89	kJ/mol	Joback Method
hf	-305.85	kJ/mol	Joback Method
hfus	22.84	kJ/mol	Joback Method
hvap	65.79	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.230		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	659.28	K	Joback Method
tc	857.10	K	Joback Method
tf	323.67	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.62	J/mol×K	659.28	Joback Method
cpg	607.64	J/mol×K	692.25	Joback Method
cpg	624.61	J/mol×K	725.22	Joback Method
cpg	640.58	J/mol×K	758.19	Joback Method
cpg	655.62	J/mol×K	791.16	Joback Method
cpg	669.79	J/mol×K	824.13	Joback Method
cpg	683.15	J/mol×K	857.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R435868&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume