bisabolene-2-ol

Inchi: InChI=1S/C15H24O/c1-11(2)6-5-7-13(4)14-9-8-12(3)10-15(14)16/h6-7,10,14-16H,5,8-9H
InchiKey: YTPHVDMIUVORDT-QPEQYQDCSA-N
Formula: C15H24O
SMILES: CC(C)=CCC=C(C)C1CCC(C)=CC1O
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	119.01	kJ/mol	Joback Method
hf	-210.01	kJ/mol	Joback Method
hfus	30.22	kJ/mol	Joback Method
hvap	66.81	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.006		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	1618.00		NIST Webbook
tb	661.88	K	Joback Method
tc	859.90	K	Joback Method
tf	297.97	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.04	J/mol×K	661.88	Joback Method
cpg	584.62	J/mol×K	694.88	Joback Method
cpg	601.23	J/mol×K	727.89	Joback Method
cpg	616.91	J/mol×K	760.89	Joback Method
cpg	631.71	J/mol×K	793.89	Joback Method
cpg	645.69	J/mol×K	826.90	Joback Method
cpg	658.90	J/mol×K	859.90	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=R239635&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