bisabolenol

Inchi: InChI=1S/C15H24O/c1-12(2)5-4-6-13(3)15-9-7-14(11-16)8-10-15/h5,7,15-16H,3-4,6,8-11
InchiKey: AWXTUFPUJSQYGO-HNNXBMFYSA-N
Formula: C15H24O
SMILES: C=C(CCC=C(C)C)C1CC=C(CO)CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	134.34	kJ/mol	Joback Method
hf	-181.46	kJ/mol	Joback Method
hfus	27.66	kJ/mol	Joback Method
hvap	66.49	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.008		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinpol	1692.00		NIST Webbook
tb	659.07	K	Joback Method
tc	853.50	K	Joback Method
tf	305.53	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.70	J/mol×K	659.07	Joback Method
cpg	580.78	J/mol×K	691.47	Joback Method
cpg	596.91	J/mol×K	723.88	Joback Method
cpg	612.15	J/mol×K	756.28	Joback Method
cpg	626.54	J/mol×K	788.69	Joback Method
cpg	640.14	J/mol×K	821.09	Joback Method
cpg	652.98	J/mol×K	853.50	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=R239640&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