«beta»-Bisabolol oxide

Inchi: InChI=1S/C15H26O2/c1-11-7-9-15(16,10-8-11)12(2)5-6-13-14(3,4)17-13/h7,12-13,16H,5
InchiKey: KSJJBQOSDNNHMT-PIMMBPRGSA-N
Formula: C15H26O2
SMILES: CC1=CCC(O)(C(C)CCC2OC2(C)C)CC1
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	-63.12	kJ/mol	Joback Method
hf	-458.87	kJ/mol	Joback Method
hfus	22.43	kJ/mol	Joback Method
hvap	68.47	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.441		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
ripol	2115.00		NIST Webbook
ripol	2115.00		NIST Webbook
tb	687.53	K	Joback Method
tc	892.17	K	Joback Method
tf	413.36	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.56	J/mol×K	687.53	Joback Method
cpg	641.60	J/mol×K	721.64	Joback Method
cpg	659.03	J/mol×K	755.74	Joback Method
cpg	676.05	J/mol×K	789.85	Joback Method
cpg	692.86	J/mol×K	823.96	Joback Method
cpg	709.65	J/mol×K	858.07	Joback Method
cpg	726.63	J/mol×K	892.17	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=R506524&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume