7-epi-«beta»-Bisabolol

Other names: (-)-epi-«beta»-bisabolol
Inchi: InChI=1S/C15H26O/c1-12(2)6-5-11-15(4,16)14-9-7-13(3)8-10-14/h6,14,16H,3,5,7-11H2,
InchiKey: AOJGKVRVMQAERF-UHFFFAOYSA-N
Formula: C15H26O
SMILES: C=C1CCC(C(C)(O)CCC=C(C)C)CC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	90.64	kJ/mol	Joback Method
hf	-267.92	kJ/mol	Joback Method
hfus	20.85	kJ/mol	Joback Method
hvap	64.99	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.230		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1658.00		NIST Webbook
ripol	2163.00		NIST Webbook
tb	654.30	K	Joback Method
tc	851.11	K	Joback Method
tf	324.07	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.75	J/mol×K	654.30	Joback Method
cpg	606.96	J/mol×K	687.10	Joback Method
cpg	624.11	J/mol×K	719.90	Joback Method
cpg	640.26	J/mol×K	752.71	Joback Method
cpg	655.45	J/mol×K	785.51	Joback Method

cpg	669.76	J/mol×K	818.31	Joback Method
cpg	683.24	J/mol×K	851.11	Joback Method

Sources

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=R226916&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume