epi- «beta»-Bisabolol

Inchi: InChI=1S/C15H26O/c1-12(2)6-5-7-14(4)15(16)10-8-13(3)9-11-15/h6,8,14,16H,5,7,9-11H
InchiKey: WTVHAMTYZJGJLJ-LOACHALJSA-N
Formula: C15H26O
SMILES: CC(C)=CCCC(C)C1(O)CC=C(C)CC1
Mol. weight [g/mol]: 222.37
CAS: 235421-59-7

Physical Properties

Property code	Value	Unit	Source
gf	47.12	kJ/mol	Joback Method
hf	-287.14	kJ/mol	Joback Method
hfus	20.43	kJ/mol	Joback Method
hvap	65.55	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.230		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	1647.00		NIST Webbook
ripol	2150.00		NIST Webbook
ripol	2128.00		NIST Webbook
ripol	2128.00		NIST Webbook
tb	662.31	K	Joback Method
tc	860.22	K	Joback Method
tf	330.15	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.91	J/mol×K	662.31	Joback Method
cpg	601.50	J/mol×K	695.29	Joback Method
cpg	618.27	J/mol×K	728.28	Joback Method
cpg	634.34	J/mol×K	761.26	Joback Method
cpg	649.80	J/mol×K	794.25	Joback Method

cpg	664.78	J/mol×K	827.23	Joback Method
cpg	679.38	J/mol×K	860.22	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=C235421597&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