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-GJZGRUSLSA-N
Formula: C15H26O
SMILES: CC(C)=CCCC(C)C1(O)CC=C(C)CC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
hfus	20.43	kJ/mol	Joback Method
hvap	79.20	kJ/mol	Cheméo Relay (1.0)
logp	4.230		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
rinpol	1672.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1672.00		NIST Webbook
ripol	1658.00		NIST Webbook

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R610227&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices