(-)-«alpha»-bisabolol

Other names: Bisabolol (isomer A)
Inchi: InChI=1S/C15H26O/c1-12(2)6-5-11-15(4,16)14-9-7-13(3)8-10-14/h6-7,14,16H,5,8-11H2,
InchiKey: RGZSQWQPBWRIAQ-GJZGRUSLSA-N
Formula: C15H26O
SMILES: CC(C)=CCCC(C)(O)C1CC=C(C)CC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
hfus	22.84	kJ/mol	Joback Method
logp	4.230		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
rinpol	1646.40		NIST Webbook
ripol	2229.00		NIST Webbook
ripol	2229.00		NIST Webbook
tb	564.91	K	Cheméo Relay (1.0)
tf	311.61	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.62	J/mol×K	659.28	Joback Method
cpg	607.64	J/mol×K	692.25	Joback Method
cpg	624.61	J/mol×K	725.22	Joback Method
cpg	640.58	J/mol×K	758.19	Joback Method
cpg	655.62	J/mol×K	791.16	Joback Method
cpg	669.79	J/mol×K	824.13	Joback Method
cpg	683.15	J/mol×K	857.10	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R329921&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point