«beta»-Bisabolen-12-ol

Other names: Bisabolen-12-ol-«beta»
Inchi: InChI=1S/C15H24O/c1-12-7-9-15(10-8-12)14(3)6-4-5-13(2)11-16/h5,7,15-16H,3-4,6,8-11
InchiKey: HBVOEGGRCJCMLG-ACAGNQJTSA-N
Formula: C15H24O
SMILES: C=C(CCC=C(C)CO)C1CC=C(C)CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
hfus	27.66	kJ/mol	Joback Method
hvap	95.23	kJ/mol	Cheméo Relay (1.0)
ie	8.41	eV	Cheméo Relay (1.0)
log10ws	-3.86		Cheméo Relay (1.0)
logp	4.008		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
rinpol	1759.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tb	589.98	K	Cheméo Relay (1.0)
tf	300.82	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.70	J/mol×K	659.07	Joback Method
cpg	580.78	J/mol×K	691.47	Joback Method
cpg	596.91	J/mol×K	723.88	Joback Method
cpg	612.15	J/mol×K	756.28	Joback Method
cpg	626.54	J/mol×K	788.69	Joback Method
cpg	640.14	J/mol×K	821.09	Joback Method
cpg	652.98	J/mol×K	853.50	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R88265&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point