cis-«beta»-sesquiphellandrol

Inchi: InChI=1S/C15H24O/c1-11(2)6-5-7-12(3)14-9-8-13(4)15(16)10-14/h6,8-9,12,14-16H,4-5,7
InchiKey: UNSGLJWOHGSVLW-ZRNAQANOSA-N
Formula: C15H24O
SMILES: C=C1C=CC(C(C)CCC=C(C)C)CC1O
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	107.61	kJ/mol	Joback Method
hf	-227.01	kJ/mol	Joback Method
hfus	27.03	kJ/mol	Joback Method
hvap	65.88	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.862		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
ripol	2396.00		NIST Webbook
tb	651.58	K	Joback Method
tc	843.66	K	Joback Method
tf	303.17	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.65	J/mol×K	651.58	Joback Method
cpg	583.04	J/mol×K	683.59	Joback Method
cpg	599.49	J/mol×K	715.61	Joback Method
cpg	615.03	J/mol×K	747.62	Joback Method
cpg	629.71	J/mol×K	779.63	Joback Method
cpg	643.56	J/mol×K	811.64	Joback Method
cpg	656.60	J/mol×K	843.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R314013&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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