«beta»-Sesquiphellandren-8-ol

Inchi: InChI=1S/C15H24O/c1-11(2)5-10-15(16)13(4)14-8-6-12(3)7-9-14/h5-6,8,13-16H,3,7,9-10
InchiKey: COLXZUVHIZOLPD-ZYOSVBKOSA-N
Formula: C15H24O
SMILES: C=C1C=CC(C(C)C(O)CC=C(C)C)CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	112.88	kJ/mol	Joback Method
hf	-211.95	kJ/mol	Joback Method
hfus	22.44	kJ/mol	Joback Method
hvap	65.81	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.862		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2005.50	kPa	Joback Method
rinpol	1524.00		NIST Webbook
tb	655.81	K	Joback Method
tc	851.34	K	Joback Method
tf	292.41	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.24	J/mol×K	655.81	Joback Method
cpg	581.52	J/mol×K	688.40	Joback Method
cpg	597.82	J/mol×K	720.99	Joback Method
cpg	613.20	J/mol×K	753.58	Joback Method
cpg	627.70	J/mol×K	786.17	Joback Method
cpg	641.35	J/mol×K	818.76	Joback Method
cpg	654.21	J/mol×K	851.34	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R412994&Units=SI

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