Germacrene B alcohol

Inchi: InChI=1S/C15H24O/c1-12-5-4-6-13(2)8-10-15(9-7-12)14(3)11-16/h5,8,16H,4,6-7,9-11H2
InchiKey: JEPRHCQQNHNKJV-MPLFWACNSA-N
Formula: C15H24O
SMILES: CC1=CCC(=C(C)CO)CCC(C)=CCC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	-0.07	kJ/mol	Joback Method
hf	-296.28	kJ/mol	Joback Method
hfus	21.74	kJ/mol	Joback Method
hvap	69.86	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.152		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinpol	1700.00		NIST Webbook
rinpol	1694.00		NIST Webbook
tb	690.88	K	Joback Method
tc	902.36	K	Joback Method
tf	340.13	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.26	J/mol×K	690.88	Joback Method
cpg	589.63	J/mol×K	726.13	Joback Method
cpg	606.85	J/mol×K	761.37	Joback Method
cpg	622.95	J/mol×K	796.62	Joback Method
cpg	637.92	J/mol×K	831.86	Joback Method
cpg	651.80	J/mol×K	867.11	Joback Method
cpg	664.59	J/mol×K	902.36	Joback Method

Sources

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=R336682&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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