Germacra-1(10),5-dien-3,4-diol

Inchi: InChI=1S/C15H26O2/c1-11(2)13-7-5-12(3)6-8-14(16)15(4,17)10-9-13/h6,9-11,13-14,16-1
InchiKey: GHCUEDNOTXRLCD-QHFJKWGLSA-N
Formula: C15H26O2
SMILES: CC1=CCC(O)C(C)(O)C=CC(C(C)C)CC1
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	-195.23	kJ/mol	Joback Method
hf	-554.34	kJ/mol	Joback Method
hfus	20.59	kJ/mol	Joback Method
hvap	82.55	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.057		Crippen Method
mcvol	214.490	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
rinpol	1704.00		NIST Webbook
rinpol	1704.00		NIST Webbook
tb	757.35	K	Joback Method
tc	958.78	K	Joback Method
tf	388.21	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.35	J/mol×K	757.35	Joback Method
cpg	684.89	J/mol×K	790.92	Joback Method
cpg	701.61	J/mol×K	824.49	Joback Method
cpg	717.57	J/mol×K	858.06	Joback Method
cpg	732.84	J/mol×K	891.64	Joback Method
cpg	747.50	J/mol×K	925.21	Joback Method
cpg	761.60	J/mol×K	958.78	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=R290214&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