(E,E)-Farnesa-1,6,9-trien-3,11-diol

Other names: 2,6,10-Trimethyldodeca-3(E),6(E),11-trien-2,10-diol
Inchi: InChI=1S/C15H26O2/c1-6-15(5,17)12-8-10-13(2)9-7-11-14(3,4)16/h6-7,10-11,16-17H,1,8
InchiKey: WPGYCMWKXXCJMW-JPTKLRQTSA-N
Formula: C15H26O2
SMILES: C=CC(C)(O)CCC=C(C)CC=CC(C)(C)O
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	47.19	kJ/mol	Joback Method
hf	-324.81	kJ/mol	Joback Method
hfus	25.77	kJ/mol	Joback Method
hvap	79.08	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.367		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	1650.00		NIST Webbook
rinpol	1648.00		NIST Webbook
ripol	2407.00		NIST Webbook
ripol	2484.00		NIST Webbook
ripol	2484.00		NIST Webbook
tb	725.38	K	Joback Method
tc	907.79	K	Joback Method
tf	359.41	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.25	J/mol×K	725.38	Joback Method
cpg	654.70	J/mol×K	755.78	Joback Method
cpg	667.44	J/mol×K	786.18	Joback Method
cpg	679.55	J/mol×K	816.58	Joback Method

cpg	691.11	J/mol×K	846.98	Joback Method
cpg	702.18	J/mol×K	877.39	Joback Method
cpg	712.86	J/mol×K	907.79	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=R232669&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume