Vetiselinenol

Other names: trans-Eudesma-4(15),7-dien-12-ol
Inchi: InChI=1S/C15H24O/c1-11-5-4-7-15(3)8-6-13(9-14(11)15)12(2)10-16/h6,12,14,16H,1,4-5
InchiKey: RQWRGJGCTMAFBS-PESDSKBTSA-N
Formula: C15H24O
SMILES: C=C1CCCC2(C)CC=C(C(C)CO)CC12
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	77.18	kJ/mol	Joback Method
hf	-243.69	kJ/mol	Joback Method
hfus	16.42	kJ/mol	Joback Method
hvap	65.75	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1704.00		NIST Webbook
rinpol	1730.00		NIST Webbook
ripol	2343.00		NIST Webbook
tb	668.44	K	Joback Method
tc	875.24	K	Joback Method
tf	377.29	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.07	J/mol×K	668.44	Joback Method
cpg	588.18	J/mol×K	702.91	Joback Method
cpg	605.40	J/mol×K	737.37	Joback Method
cpg	621.84	J/mol×K	771.84	Joback Method
cpg	637.63	J/mol×K	806.31	Joback Method
cpg	652.89	J/mol×K	840.77	Joback Method

cpg	667.74	J/mol×K	875.24	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=R199314&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume