Cembra-2,7,11-trien-4-ol

Inchi: InChI=1S/C20H34O/c1-16(2)19-12-11-18(4)9-6-8-17(3)10-7-14-20(5,21)15-13-19/h9-10,
InchiKey: YAPXSYXFLHDPCK-MXUGJEEPSA-N
Formula: C20H34O
SMILES: CC1=CCCC(C)(O)C=CC(C(C)C)CCC(C)=CCC1
Mol. weight [g/mol]: 290.48

Physical Properties

Property code	Value	Unit	Source
gf	-36.67	kJ/mol	Joback Method
hf	-463.30	kJ/mol	Joback Method
hfus	20.82	kJ/mol	Joback Method
hvap	78.95	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	5.813		Crippen Method
mcvol	274.770	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinpol	2057.00		NIST Webbook
rinpol	2057.00		NIST Webbook
tb	805.46	K	Joback Method
tc	1028.60	K	Joback Method
tf	387.18	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.52	J/mol×K	805.46	Joback Method
cpg	900.62	J/mol×K	842.65	Joback Method
cpg	922.31	J/mol×K	879.84	Joback Method
cpg	942.67	J/mol×K	917.03	Joback Method
cpg	961.78	J/mol×K	954.22	Joback Method
cpg	979.69	J/mol×K	991.41	Joback Method
cpg	996.50	J/mol×K	1028.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R332551&Units=SI
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

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