(1R,3S)-cembra-4,7,11,15-tetraen-3-ol

Inchi: InChI=1S/C20H32O/c1-15(2)19-13-12-17(4)9-6-8-16(3)10-7-11-18(5)20(21)14-19/h9-11,
InchiKey: JMLCJQLPSRCUBV-PJRVNRGZSA-N
Formula: C20H32O
SMILES: C=C(C)C1CCC(C)=CCCC(C)=CCC=C(C)C(O)C1
Mol. weight [g/mol]: 288.47

Physical Properties

Property code	Value	Unit	Source
gf	40.92	kJ/mol	Joback Method
hf	-369.09	kJ/mol	Joback Method
hfus	27.66	kJ/mol	Joback Method
hvap	80.56	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.733		Crippen Method
mcvol	270.470	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
rinpol	2192.00		NIST Webbook
tb	807.20	K	Joback Method
tc	1027.70	K	Joback Method
tf	375.08	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.18	J/mol×K	807.20	Joback Method
cpg	875.34	J/mol×K	843.95	Joback Method
cpg	894.62	J/mol×K	880.70	Joback Method
cpg	911.99	J/mol×K	917.45	Joback Method
cpg	927.44	J/mol×K	954.20	Joback Method
cpg	940.95	J/mol×K	990.95	Joback Method
cpg	952.51	J/mol×K	1027.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418907&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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