cis-abienol

Inchi: InChI=1S/C20H34O/c1-7-15(2)9-10-17-19(5)13-8-12-18(3,4)16(19)11-14-20(17,6)21/h7,9
InchiKey: ZAZVCYBIABTSJR-DHDCSXOGSA-N
Formula: C20H34O
SMILES: C=CC(C)=CCC1C(C)(O)CCC2C(C)(C)CCCC21C
Mol. weight [g/mol]: 290.48

Physical Properties

Property code	Value	Unit	Source
gf	173.71	kJ/mol	Joback Method
hf	-269.84	kJ/mol	Joback Method
hfus	21.45	kJ/mol	Joback Method
hvap	72.30	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.502		Crippen Method
mcvol	268.210	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	2150.00		NIST Webbook
rinpol	2111.00		NIST Webbook
rinpol	2111.00		NIST Webbook
rinpol	2128.00		NIST Webbook
tb	767.17	K	Joback Method
tc	979.48	K	Joback Method
tf	435.96	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.65	J/mol×K	767.17	Joback Method
cpg	880.12	J/mol×K	802.55	Joback Method
cpg	903.54	J/mol×K	837.94	Joback Method
cpg	927.22	J/mol×K	873.32	Joback Method
cpg	951.49	J/mol×K	908.71	Joback Method
cpg	976.65	J/mol×K	944.09	Joback Method

cpg	1003.03	J/mol×K	979.48	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=R167189&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume