Isoabienol

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/h7,1
InchiKey: JTWQQJDENGGSBJ-KOQQBVACSA-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	181.33	kJ/mol	Joback Method
hf	-261.63	kJ/mol	Joback Method
hfus	19.96	kJ/mol	Joback Method
hvap	71.67	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.502		Crippen Method
mcvol	268.210	ml/mol	McGowan Method
pc	1524.69	kPa	Joback Method
rinpol	2107.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2078.00		NIST Webbook
ripol	2606.00		NIST Webbook
ripol	2606.00		NIST Webbook
tb	759.69	K	Joback Method
tc	968.49	K	Joback Method
tf	439.28	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.43	J/mol×K	759.69	Joback Method
cpg	877.58	J/mol×K	794.49	Joback Method
cpg	900.58	J/mol×K	829.29	Joback Method
cpg	923.73	J/mol×K	864.09	Joback Method
cpg	947.32	J/mol×K	898.89	Joback Method

cpg	971.64	J/mol×K	933.69	Joback Method
cpg	996.99	J/mol×K	968.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202950&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume