cis-ferruginol

Inchi: InChI=1S/C20H30O/c1-13(2)15-11-14-7-8-18-19(3,4)9-6-10-20(18,5)16(14)12-17(15)21/
InchiKey: QXNWVJOHUAQHLM-ICSRJNTNSA-N
Formula: C20H30O
SMILES: CC(C)c1cc2c(cc1O)C1(C)CCCC(C)(C)C1CC2
Mol. weight [g/mol]: 286.45

Physical Properties

Property code	Value	Unit	Source
gf	132.22	kJ/mol	Joback Method
hf	-281.71	kJ/mol	Joback Method
hfus	23.62	kJ/mol	Joback Method
hvap	73.90	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	5.546		Crippen Method
mcvol	253.050	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2362.00		NIST Webbook
rinpol	2371.00		NIST Webbook
tb	791.65	K	Joback Method
tc	1034.71	K	Joback Method
tf	535.74	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.54	J/mol×K	791.65	Joback Method
cpg	831.05	J/mol×K	832.16	Joback Method
cpg	854.62	J/mol×K	872.67	Joback Method
cpg	878.69	J/mol×K	913.18	Joback Method
cpg	903.66	J/mol×K	953.69	Joback Method
cpg	929.95	J/mol×K	994.20	Joback Method

cpg	957.98	J/mol×K	1034.71	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R241613&Units=SI

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