Phyllocladanol

Inchi: InChI=1S/C20H34O/c1-17(2)9-5-10-18(3)15(17)8-11-20-12-14(6-7-16(18)20)19(4,21)13-
InchiKey: FZSRMADKTOBCNT-UHFFFAOYSA-N
Formula: C20H34O
SMILES: CC1(C)CCCC2(C)C1CCC13CC(CCC12)C(C)(O)C3
Mol. weight [g/mol]: 290.48

Physical Properties

Property code	Value	Unit	Source
gf	130.21	kJ/mol	Joback Method
hf	-341.86	kJ/mol	Joback Method
hfus	13.80	kJ/mol	Joback Method
hvap	71.60	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	5.170		Crippen Method
mcvol	255.090	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook
tb	780.17	K	Joback Method
tc	1008.89	K	Joback Method
tf	516.54	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.24	J/mol×K	780.17	Joback Method
cpg	899.87	J/mol×K	818.29	Joback Method
cpg	927.16	J/mol×K	856.41	Joback Method
cpg	955.65	J/mol×K	894.53	Joback Method
cpg	985.88	J/mol×K	932.65	Joback Method
cpg	1018.38	J/mol×K	970.77	Joback Method
cpg	1053.70	J/mol×K	1008.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R614492&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