cis-Totarol, methyl ether

Inchi: InChI=1S/C21H32O/c1-14(2)19-15-8-11-18-20(3,4)12-7-13-21(18,5)16(15)9-10-17(19)22
InchiKey: DORDKDUSCNWFPJ-ZYZRXSCRSA-N
Formula: C21H32O
SMILES: COc1ccc2c(c1C(C)C)CCC1C(C)(C)CCCC21C
Mol. weight [g/mol]: 300.48

Physical Properties

Property code	Value	Unit	Source
gf	180.63	kJ/mol	Joback Method
hf	-268.73	kJ/mol	Joback Method
hfus	21.23	kJ/mol	Joback Method
hvap	66.18	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	5.849		Crippen Method
mcvol	267.140	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
rinpol	2205.00		NIST Webbook
rinpol	2205.00		NIST Webbook
tb	761.31	K	Joback Method
tc	991.05	K	Joback Method
tf	470.04	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.37	J/mol×K	761.31	Joback Method
cpg	854.48	J/mol×K	799.60	Joback Method
cpg	878.05	J/mol×K	837.89	Joback Method
cpg	901.37	J/mol×K	876.18	Joback Method
cpg	924.73	J/mol×K	914.47	Joback Method
cpg	948.41	J/mol×K	952.76	Joback Method
cpg	972.69	J/mol×K	991.05	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=R329609&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