cis-Totarol

Inchi: InChI=1S/C20H30O/c1-13(2)18-14-7-10-17-19(3,4)11-6-12-20(17,5)15(14)8-9-16(18)21/
InchiKey: ZRVDANDJSTYELM-PXNSSMCTSA-N
Formula: C20H30O
SMILES: CC(C)c1c(O)ccc2c1CCC1C(C)(C)CCCC21C
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	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
rinpol	2276.00		NIST Webbook
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
rinpol	2257.00		NIST Webbook
rinpol	2230.00		NIST Webbook
rinpol	2276.00		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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R301938&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

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