Turmerol isomer Unknown

Inchi: InChI=1S/C15H22O/c1-11(2)9-15(16)10-13(4)14-7-5-12(3)6-8-14/h5-9,13,15-16H,10H2,1
InchiKey: NRBFEAZFHRHFFQ-UHFFFAOYSA-N
Formula: C15H22O
SMILES: CC(C)=CC(O)CC(C)c1ccc(C)cc1
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	108.17	kJ/mol	Joback Method
hf	-183.23	kJ/mol	Joback Method
hfus	24.19	kJ/mol	Joback Method
hvap	67.86	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.816		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1637.10		NIST Webbook
rinpol	1637.10		NIST Webbook
tb	669.60	K	Joback Method
tc	868.62	K	Joback Method
tf	309.53	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.39	J/mol×K	669.60	Joback Method
cpg	554.94	J/mol×K	702.77	Joback Method
cpg	569.60	J/mol×K	735.94	Joback Method
cpg	583.42	J/mol×K	769.11	Joback Method
cpg	596.45	J/mol×K	802.28	Joback Method
cpg	608.75	J/mol×K	835.45	Joback Method
cpg	620.35	J/mol×K	868.62	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=U412349&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